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# **YUCOMAT 2011**

THIRTEENTH ANNUAL CONFERENCE

Herceg Novi, Montenegro, September 5–9, 2011 http://www.mrs-serbia.org.rs



# Programme and The Book of Abstracts

Organised by:

**Materials Research Society of Serbia** 

under the auspices of

Federation of European Materials Societies (FEMS)

nd

Materials Research Society (MRS)

#### THIRTEENTH ANNUAL CONFERENCE

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Hunguest Hotel Sun Resort Herceg Novi, Montenegro, September 5-9, 2011 http://www.mrs-serbia.org.rs

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Title: THE THIRTEENTH ANNUAL CONFERENCE

YUCOMAT 2011

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#### THIRTEENTH ANNUAL CONFERENCE "YUCOMAT 2011"

Herceg Novi, September 5-9, 2011

#### WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA

My Esteemed Colleagues,



I will start with one simple Welcome to the XIII YUCOMAT! Let me express my hopes that this will be yet another YUCOMAT where thoughts on science and technology will be mingled with and fertilized by an inspiring, summery ambiance and where new generations of scientific thinkers will coalesce with the elderly and experienced ones.

Intensive communication between the developing countries and the developed ones is of crucial importance for the progress of both. For, affluent social islands surrounded by all but prosperous milieus have been over and over again shown as unsustainable. To ensure the thriving

of the developed world, therefore, its eyes should be kept on assisting the small ones in their progress. On the other hand, some of the most remarkable scientific discoveries are known to have stemmed from miniscule funding, as pointed out these days by historians of science. Modest research environments, such as those existing in many small countries, are thus often thought to be fertile grounds for the invention of simple and yet extraordinarily efficient and eco-friendly methods and approaches. YUCOMAT, in fact, originated from the idea that a scientific community of a small country - such as all former Yugoslav countries were in 1995 and still are - would greatly benefit from a meeting whereat local and worldly renowned researchers would present their exciting findings side by side. Today, sixteen years later we witness this idea to still flourish in reality as we have gathered here now for the 13<sup>th</sup> time for one such occasion.

This year's YUCOMAT is nowhere different from the previous years' ones in terms of its size, with 155 posters and 86 lectures that are scheduled to be presented by participants from more than 30 countries of the world during the 5 days of the conference. Presentations are divided to 5 symposia and, also, number of lectures that are to be held by 26 plenary lecturers this year is more than we had any time before.

Just as every year before, this year as well we offer you a similar program both inside and outside of the lecture and exhibition halls. There is one major new thing, however, as some of you must have noticed: namely, the venue that hosts the conference. Instead of Hotel Plaza in the past, this year it is Hunguest Sun Resort. Aside from it, the welcome cocktail will again be held on Monday, that is, later in the day; poster sessions will take place during the evening hours from Tuesday to Thursday; an organized excursion to Dubrovnik is on Wednesday afternoon; a boat-trip around the Bay on Thursday afternoon, and a plenty of coffee breaks will be scattered throughout the days as an opportunity to relax, network and socialize. During this Opening Ceremony we will recognize the winners of the best PhD and Master of Science theses defended between this and the previous YUCOMAT, while during the Closing Ceremony we will also announce the best oral and poster presenters. In the back of the lecture hall also a small exhibition fair will be held throughout the course of the conference.

The topics presented on during this year's YUCOMAT are the same ones that are considered "hot" in the circles of international experts in the field. A rigorous selection of abstracts has been implemented and invitations for plenary lectures were sent to carefully chosen and recommended scientists who have done a great deal of research in their fields so as to keep the program of this year's YUCOMAT concordant with the latest trends. Like every other aspect of

the scientific and social world of ours, materials science has undergone a tremendous change in trends over the course of time. What was all the rage two decades ago might be only a minor, sideway field at this point of time. To keep abreast with this process of change, the scientists have to be constantly updated with the cutting-edge research that takes place in quite often distant places on the globe. Scientific journals and Internet presentations nowadays do offer a glimpse into exciting new research; however, the chance to meet in person the presenters who are experts in their fields, ranging from nanomaterials to bioengineering to soft matter to semiconductors and photonics, and feel their science from a very intimate angle is still the privilege of participants of conferences of this nature.

To wrap things up, on behalf of the MRS-Serbia Officers, the Organizing Committee, the International Advisory Board and Sasha, our Conference Secretary, which I all greatly acknowledge for their efforts in putting up this entire meeting, I would like to express delight over the great amount of interest in participation at this year's YUCOMAT. From a conference organized for the first time in a country falling apart under the pressure of the civil war to one used in international circles as a model for a successful small country's scientific meeting, it has undergone a tremendous change for better over years. We wish to continue this trend of success and sustain in our mission, which, as I mentioned earlier, is to connect the scientific body of a small and developing country with those of developed ones for the benefit of the entire planet. Having the YUCOMAT happen year after year reminds me that we are making the steps to better the world by our sciences and this is the reward for not only us, the organizers, but all the more for you, the attendees of this wonderful meeting.

I wish you a splendid time during these YUCOMAT days!

Dragan Uskokovic

#### THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

#### MRS-Serbia

President: Dragan Uskoković

Vice-presidents: Slobodan Milonjić, Velimir Radmilović, Dejan Raković

General Secretary: Jovan Nedeljković

Members: Snežana Bošković, Milorad Davidović, Vera Dondur, Nenad Ignjatović, Djuro Koruga, Nedeljko Krstajić, Slavko Mentus, Zoran Petrović, Milenko Plavšić, Zoran Popović, Vladimir Srdić,

Momčilo Stevanović, Jovan Šetrajčić, Miodrag Zlatanović

#### **International Advisory Board**

Chair: Robert Sinclair (USA)

Members: Fritz Aldinger (Germany), Rostislav A. Andrievski (Russia), Aline Auroux (France), Djamila Bahloul-Hourlier (France), Xavier Batlle (Spain), Serena Best (UK), Ivan Božović (USA), Philippe Colomban (France), Uli Dahmen (USA), Miha Drofenik (Slovenia), Michel Fedoroff (France), Mauro Ferrari (USA), Horst Hahn (Germany), Paul Harrison (UK), Felix T. Hong (USA), Robert Hull (USA), Wolfgang Jaeger (Germany), Thomas Jung (Switzerland), Josè M. Kenny (Italy), Alexander H. King (USA), Vladimir Krstić (Canada), Toshiaki Makabe (Japan), Egon Matijević (USA), Amelia Montone (Italy), Eiji Osawa (Japan), Zoran S. Petrović (USA), Robert Ritchie (USA), Frances Ross (USA), Richard W. Siegel (USA), Mamoru Senna (Japan), Valeriy V. Skorohod (Ukraine), Danilo Suvorov (Slovenia), Enrico Traversa (Italy), Jose A. Varela (Brazil), Gordana Vunjak Novaković (USA)

#### **Conference Organising Committee**

Chairperson: Mira Vukčević

**Members:** Nikola Cvjetićanin, Kemal Delijić, Branko Matović, Jovan Mirković, Nebojša Mitrović, Željka Nikitović, Nebojša Romčević, Edin Suljovrujić, Ljiljana Živković

Conference Secretary: Aleksandra Stojičić

#### **HISTORY:**

Materials science and engineering incorporate acquiring of knowledge on synthesis and processing of materials, their composition and structure, properties and behaviour, functions and potentialities as well as application of that knowledge to various final products. Economic prosperity, life quality, and healthy environment are tightly connected with the improvements in the existing and the development of new materials and processing technologies. These improvements and development can contribute greatly to the national priorities: energy saving, environment and health protection, information and communication, infrastructure, transportation, etc.

The First Conference on materials science and engineering, including physics, physical chemistry, condensed matter chemistry, and technology in general, was held in September 1995, in Herceg Novi. An initiative to establish Yugoslav Materials Research Society was born at the conference and, similar to other MR societies in the world, the programme was made and objectives determined. The Yugoslav Materials Research Society (Yu-MRS), a non-government and non-profit scientific association, was founded in 1997 to promote multidisciplinary goal-oriented research in materials science and engineering. Main task and objective of the Society is to encourage creativity in materials research and engineering to reach a harmonic coordination between achievements in this field in our country and analogous activities in the world with an aim to include our country into the global international projects. Until 2003, Conferences were held every second year and then they grew into Annual Conferences that were traditionally held in Herceg Novi in September of every year. Following the political separation between Serbia and Montenegro, in 2007 Yu-MRS formed two new MRS: MRS-Serbia (official successor of Yu-MRS) and MRS-Montenegro (in founding). In 2008 MRS-Serbia became a member of FEMS (Federation of European Materials Societies).

## THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

#### GENERAL INFORMATION

**DATE AND VENUE:** The conference will be held on September 5-9, 2011, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 5, at 09.00 and end on Friday, September 9<sup>th</sup>, 2011, at 11.30.

**REGISTRATION:** Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk (Conference Secretariat) open on Sunday, September 4, Monday, September 5, and Tuesday, September 6, from 8.00 to 19.00, on Wednesday and Thursday 8.00-13.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their advance registration fee payment and their registration form.

**INSTRUCTION FOR AUTHORS:** The conference will feature plenary sessions, oral sessions, poster sessions, and an Exhibition of synthesis and characterization equipment.

Time of papers' presentations to be given in ORAL SESSIONS is limited. Time available for delivery is 30 min for plenary and 15 min for other papers including discussion (5-10 min). Video-beam is available. PowerPoint presentations, recorded on CD or memo-stick, should be given at registration. In POSTER SESSIONS, the authors are requested to display their papers minimum two hours before the session and to be present beside their posters during the session. Poster sessions are held in Chieldren Play Center (by the pool) which is open Tuesday to Thursday 18.00-22.00.

**CONFERENCE AWARDS:** Materials Research Society of Serbia will award the authors (preferable young members under 35) of the best oral and poster presentation at the conference, and also the authors of highly rated PhD and MSc theses defended between two conferences. Awarded researchers are granted free registration at the next YUCOMAT Conference.

**ADDITIONAL ACTIVITIES:** An Exhibition of synthesis and characterization equipment will be held during the Conference. Traditional Cocktail Party on Monday evening and excursions on Wednesday afternoon to Dubrovnik (Croatia) and Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

# Programme

#### GENERAL CONFERENCE PROGRAMME

SYMPOSIUM A: Advanced Methods in Synthesis

SYMPOSIUM B: Advanced Materials for High-

technologies

SYMPOSIUM C: Nanostructured Materials SYMPOSIUM D: Eco-materials and Eco-

SYMPOSIUM E: Biomaterials

and Processing of Materials

Technology Application

Sunday, September 4, 2011

 $08^{00}$ - $19^{00}$  Registration

Monday, September 5, 2011

 $08^{00}$ - $09^{00}$  Registration

09<sup>00</sup> **OPENING CEREMONY** 

- Introduction and Welcome

10<sup>00</sup>-13<sup>30</sup> First Plenary Session

14<sup>00</sup> Photo Session

15<sup>00</sup>-18<sup>45</sup> Symposium A, Conference Hall

15<sup>00</sup>-18<sup>30</sup> Symposium B, Small Hall

19<sup>30</sup>-21<sup>00</sup> Cocktail Party

Tuesday, September 6, 2011

09<sup>00</sup>-13<sup>30</sup> **Second Plenary Session** 

15<sup>00</sup>-19<sup>00</sup> Symposium C, Session I, Conference Hall

15<sup>00</sup>-18<sup>30</sup> **Symposium C, Session II, Small Hall** 

20<sup>30</sup>-22<sup>00</sup> **Poster Session I** (Symposium A)

Wednesday, September 7, 2011

09<sup>00</sup>-13<sup>00</sup> Third Plenary Session

14<sup>00</sup>-19<sup>00</sup> Excursion to Dubrovnik, Croatia 20<sup>30</sup>-22<sup>00</sup> Poster Session II (Symposium B)

Thursday, September 8, 2011

09<sup>00</sup>-12<sup>30</sup> Fourth Plenary Session

14<sup>00</sup>-19<sup>00</sup> Boat-trip around Boka Kotorska Bay

20<sup>30</sup>-22<sup>00</sup> **Poster Session III** (Symposiums C, D and E)

Friday, September 9, 2011

09<sup>00</sup>-11<sup>00</sup> **Symposium E** 

11<sup>00</sup>-11<sup>30</sup> Awards and Closing of the Conference

#### FIRST PLENARY SESSION

Monday, September 5, 2011

**Session I:**  $10^{00}$ - $13^{30}$ 

Chairmen: R. Sinclair, U. Dahmen and V. Radmilović

Conference Hall

## 10<sup>00</sup>-10<sup>30</sup> NANOSTRUCTURE PROCESSING OF ADVANCED BIOMATERIALS AND BIOSYSTEMS

J.Y. Ying

Institute of Bioengineering and Nanotechnology, The Nanos, Singapore

# 10<sup>30</sup>-11<sup>00</sup> USING THE TEAM MICROSCOPE TO INVESTIGATE THE ATOMIC STRUCTURE OF PARTICLES, DEFECTS AND INTERFACES IN MATERIALS

U. Dahmen

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, University of California, One Cyclotron Rd., Berkeley, CA, USA

## 11<sup>00</sup>-11<sup>30</sup> CHARACTERIZATION AND APPLICATION OF GRAPHENE AND NANOSTRUCTURED BORON NITRIDE

A. Zettl

Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Break: 1130-1200

#### 12<sup>00</sup>-12<sup>30</sup> **BIOMIMETICS: LESSONS FROM NATURE**

B. Bhushan

Nanoprobe Laboratory for Bio- & Nanotechnology and Biomimetics, The Ohio State University, Columbus, Ohio, USA

#### 12<sup>30</sup>-13<sup>00</sup> AN UP-DATE ON FACILITIES FOR NANOCHARACTERIZATION

R. Sinclair, R.W. Chin, A.L. Koh

Department of Materials Science and Engineering and Stanford Nanocharacterization Laboratory, Stanford University, Stanford, CA, USA

## THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

13<sup>00</sup>-13<sup>30</sup> M<sub>2</sub>O<sub>3</sub>(ZnO)<sub>n</sub> NANOWIRES FOR THERMOELECTRIC APPLICATIONS

V.R. Radmilovic<sup>1,2</sup>, S.C. Andrews<sup>3,4</sup>, M.A. Fardy<sup>3,4</sup>, M.C. Moore<sup>3,4</sup>, P. Yang<sup>3,4</sup>

Nanotechnology and Functional Materials Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, <sup>2</sup>National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA, USA, <sup>3</sup>Department of Chemistry, University of California, Berkeley, CA, USA, <sup>4</sup>Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Break: 13<sup>30</sup>-15<sup>00</sup>

## SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

Monday, September 5, 2011

**Session I**: 15<sup>00</sup>-18<sup>45</sup>

Chairpersons: J. Nedeljković and N. Pankrushina

Conference Hall

## $15^{00}$ - $15^{15}$ SONOELECTROCHEMISTRY – A VERSATILE TOOL FOR THE PREPARATION OF NANOMATERIALS

Chr. Argirusis<sup>1,2</sup>, S. Martens<sup>2</sup>, P. Sakkas<sup>1</sup>, G. Sourkouni<sup>2,3</sup>, O. Schneider<sup>2,4</sup>

National Technical University of Athens; School of Chemical Engineering,
Zografou, Greece, <sup>2</sup>Clausthal University of Technology, Institute of Metallurgy,
Clausthal-Zellerfeld, Germany, <sup>3</sup>Clausthal University of Technology, Energy
Research Centre Lower Saxony, Goslar, Germany, <sup>4</sup>Technische Universität
München, Department of Physics, Chair for Energy Conversion and Storage,
Garching, Germany

15<sup>15</sup>-15<sup>30</sup> SYNTHESES AND CHARACTERIZATIONS OF LifePO<sub>4</sub> POWDERS

D. Jugović<sup>1</sup>, M. Kuzmanović<sup>1</sup>, M. Mitrić<sup>2</sup>, N. Cvjetićanin<sup>3</sup>, D. Uskoković<sup>1</sup>

Institute of Technical Sciences of the SASA, Belgrade, Serbia,

<sup>2</sup>The Vinča Institute of Nuclear Sciences, University of Belgrade, Serbia,

<sup>3</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia

## 15<sup>30</sup>-15<sup>45</sup> LITHIUM IRON PHOSPHATE MESOCRYSTALS FOR LITHIUM–ION BATTERIES

J. Popović, M. Antonietti, M.-M. Titirici
Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

## 15<sup>45</sup>-16<sup>00</sup> SINTERING OF DEFECT-FREE FUNCTIONALLY GRADED BIOMATERIALS

S. Marković<sup>1</sup>, M. Lukić<sup>1</sup>, S.D. Škapin<sup>2</sup>, D. Uskoković<sup>1</sup>

Institute of Technical Sciences of SASA, Belgrade, Serbia,

Jožef Stefan Institute, Ljubljana, Slovenia

# 16<sup>00</sup>-16<sup>15</sup> MECHANOCHEMICAL SULPHIDIZATION AND SULPHUR COATING OF NON-FERROUS METAL-OXIDES IN FLY-ASH AND THEIR RECOVERY BY FLOTATION

Q. Zhang, J. Wang, <u>F. Saito</u> IMRAM, Tohoku University, Japan

## THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

## 16<sup>15</sup>-16<sup>30</sup> THE <sup>57</sup>FE-O COMPLEXES – MÖSSBAUER PROBES TO STUDY NANOSTRUCTURED MATERIALS

E.P. Elsukov, A.V. Protasov, L.V. Dobysheva, A.K. Arzhnikov, E.V. Voronina *Physical-Technical Institute UrB RAS, Izhevsk, Russia* 

## 16<sup>30</sup>-16<sup>45</sup> NANOPOROUS ANODIC ALUMINA FILMS: INVESTIGATION OF GROWTH AND MORPHOLOGY EVOLUTION

Y. Dzhulay<sup>1</sup>, V. Kruchinin<sup>2</sup>, B. Bokhonov<sup>3</sup>, N. Uvarov<sup>1,3</sup>

Novosibirsk State University, Novosibirsk, Russia, <sup>2</sup>Institute of Semiconductor Physics SB RAS, Novosibirsk, Russia, <sup>3</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

## 16<sup>45</sup>-17<sup>00</sup> **EVAPORATION FROM LIQUID FILMS IN SOLID-LIQUID-GAS SYSTEMS** A.P. Malygin, <u>D.V. Alexandrov</u>

Department of Mathematical Physics, Urals State University, Ekaterinburg, Russia

Break: 1700-1730

## 17<sup>30</sup>-17<sup>45</sup> SOLVENT-FREE MICROWAVE ASSISTED SYNTHESES OF AMINO ACID DERIVATIVES

N.A. Pankrushina, A.N. Mikheev, M.O. Korotkih, A.V. Arzhannikov, M.K.A. Thomm

Novosibirsk State University, Novosibirsk, Russia

## $17^{45}\text{--}18^{00}$ SYNTHESIS AND CHARACTERIZATION OF $\text{Hf}_{1\text{--}x}Y_xO_{2\text{--}\delta}$ SOLID SOLUTION NANOCRYSTALS

<u>B. Matović</u>, B. Babić<sup>1</sup>, J. Pantić<sup>1</sup>, M. Pekrajski<sup>1</sup>, D. Bučevac<sup>1</sup>, M. Radović<sup>2</sup>, Z. Mitrović-Dohčević<sup>2</sup>

<sup>1</sup>Institute of Nuclear Sciences Vinča, Belgrade, Serbia, Belgrade University <sup>2</sup>Institute for Physics, Pregrevica, Belgrade, Serbia, Belgrade University

## 18<sup>00</sup>-18<sup>15</sup> "MECHANOCHEMICAL" NANO-Si METHODS OF PREPARATION, DEFECT STRUCTURE AND REACTIVITY

A.N.Streletskii, I.V.Kolbanev, A.B.Borunova, V.A. Radzig *Institute of Chemical Physics RAS, Moscow, Russia* 

#### 18<sup>15</sup>-18<sup>30</sup> SELECTIVE MICROWAVE HEATING OF COMPOUNDS, INTERCALATED INTO THE INTERLAYER SPACE OF POLIFLUORODICARBON

A.N. Mikheev, A.V. Arzhannikov, V.G. Makotchenko, M.K.A. Thomm *Novosibirsk State University, Novosibirsk, Russia* 

## $18^{30}\text{-}18^{45}$ SIZE EFFECT FOR MODEL Ag/HOPG CATALYSTS IN THE REACTION OF ETHYLENE EPOXIDATION

<u>I.P. Prosvirin</u>, D.V. Demidov, A..M. Sorokin, V.I. Bukhtiyarov *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia* 

## SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

Monday, September 5, 2011

**Session I**: 15<sup>00</sup>-18<sup>30</sup>

Chairpersons: M. Zlatanović and I. Uvarova

Small Hall

# 15<sup>00</sup>-15<sup>15</sup> THE RELAXATIONAL MODEL OF DOUBLE ELECTRIC LAYER IN DISTURBED CRYSTAL POTENTIAL RELIEF ON SUPERIONIC/ ELECTRONIC CONDUCTOR POLARIZED HETEROJUNCTIONS

A.L. Despotuli, A. V. Andreeva

Institute of Microelectronics Technology Russian Academy of Sciences (IMT RAS), Chernogolovka, Moscow Region, Russia

# 15<sup>15</sup>-15<sup>30</sup> THE INTERFACES IN SUPERIONIC CONDUCTORS AS NEW SENSITIVE MATERIAL FOR PERFORMANCE OPTIMIZATION OF NANOIONIC DEVICES

A.V. Andreeva, A.L. Despotuli

Institute of Microelectronics Technology, Russian Academy of Sciences Chernogolovka, Moscow Region, Russia

## 15<sup>30</sup>-15<sup>45</sup> **DEVELOPMENT OF BORON HYDRIDES MATERIALS FOR HYDROGEN STORAGE**

V.I. Simagina, O.V. Netskina, O.V. Komova, A.M. Ozerova, V. Odegova Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

## 15<sup>45</sup>-16<sup>00</sup> THE STUDY OF THE INTERFACIAL COATINGS ON REINFORCED CARBON AND SIC FIBERS FOR HIGH-TEMPERATURE COMPOSITES

N. Baklanova

Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russian Federation

## 16<sup>00</sup>-16<sup>15</sup> ALUMINOSILICATE INORGANIC POLYMERS: THE EFFECTS OF POLYPROPYLENE FILLERS ON MECHANICAL BEHAVIOR

L. Benešová, J. Kotek

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague 6, Czech Republic

## 16<sup>15</sup>-16<sup>30</sup> STRUCTURAL TRANSFORMATION IN La<sub>1-x</sub>Ca<sub>x</sub>MeO<sub>3</sub> (Me=Mn, Fe) PEROVSKITES DURING METHANE OXIDATION PROCESS

L.A. Isupova, S.V. Tsybulya, E.Yu. Gerasimov, V.I. Zaikovskii Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

16<sup>30</sup>-16<sup>45</sup> THERMOCHEMICAL PROPERTIES OF ZIRCONIUM, MOLYBDENUM, VANADIUM AND CHROMIUM ALUMINIDES

V.M. Chumarev<sup>1</sup>, L.Y. Udoeva<sup>1</sup>, A.V. Larionov<sup>1</sup>, M.V. Trubachev<sup>2</sup>, M.N. Baklanov<sup>2</sup>

<sup>1</sup>Institute of Metallurgy of Ural Division of Russian Academy of Sciences,

Yekaterinburg, Russia, <sup>2</sup>JSC "URALREDMET", Verkhnyaya Pyshma, Sverdlovsk

Region, Russia

 $16^{45}$ - $17^{00}$  THERMOCHEMICAL SYNTHESIS OF ALUMINIUM-VANADIUM-NITROGEN ALLOYS UNDER THE NITROGEN ATMOSPHERE

A.V. Larionov, V.M. Chumarev, R.I. Gulyaeva, S.V. Zhidovinova Institute of Metallurgy of Ural Division of Russian Academy of Sciences, Yekaterinburg, Russia

Break: 1700-1730

17<sup>30</sup>-17<sup>45</sup> SYNERGETIC EFFECT IN THE LaFeO<sub>3</sub>-CeO<sub>2</sub> SYSTEM TOWARDS CATALYTIC ACTIVITY IN HIGH TEMPERATURE REACTIONS WITH OXYGEN PARTICIPATION

L.G. Pinaeva, D.V. Ivanov, E.M. Sadovskaya, I.P. Prosvirin, L.A. Isupova Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

17<sup>45</sup>-18<sup>00</sup> SIZE EFFECT UNDER PHORETIC COATINGS PREPARATION

<u>I. Uvarova</u>, O. Shchevchenko, I. Kud

Frantsevych Institute for Problems of Materials Science of NAS of Ukraine, Kyiv,

Ukraine

 $18^{00}\text{-}18^{15}$  PHASE RELATIONS AND ADVANCED MATERIALS IN THE ZrO\_2(HfO\_2)- Y\_2O\_3-Sm\_2O\_3 SYSTEMS

E.R. Andrievskaya, V.O. Zgurovets

Institute of Materials Science Problems, National Ukrainian Academy of Sciences, Kiev, Ukraine

18<sup>15</sup>-18<sup>30</sup> MATERIAL BEHAVIOR AT THE PRE-FRACTURE STAGE AND A NEW METHOD FOR ESTIMATING THE PLASTICITY MARGIN OF MATERIALS WORKED BY PRESSING

V.I. Danilov, L.B. Zuev, D.V. Orlova, N.A. Ploskov Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia

#### SECOND PLENARY SESSION

Tuesday, September 6, 2011

**Session II:** 09<sup>00</sup>-13<sup>30</sup>

Chairmen: M. Senna, D. Suvorov and D. Raković

Conference Hall

09<sup>00</sup>-09<sup>30</sup> CHANGE IN THE CHEMICAL AND ELECTRONIC PROPERTIES OF OXIDE NANOPARTICLES BY SOLID STATE REACTIONS AT THE BOUNDARIES TO ORGANIC CRYSTALS

M. Senna

Faculty of Science and Technology, Keio University, Yokohama, Japan

09<sup>30</sup>-10<sup>00</sup> INFRARED STUDY OF SOFT CONDENSED MATTER

L. Forró

Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

10<sup>00</sup>-10<sup>30</sup> **DOPING, STRAINS AND ELECTRIC FIELD EFFECT ON SUPERCONDUCTIVITY IN ULTRA-THIN CUPRATE FILMS** 

D. Pavuna

Swiss Federal Institute of Technology (EPFL), Physics of Complex Matter, Station 3, Lausanne, Switzerland

10<sup>30</sup>-11<sup>00</sup> UNDERSTANDING THE MECHANISMS OF CARBON NANOTUBE GROWTH TERMINATION USING REAL TIME ENVIRONMENTAL TRANSMISSION ELECTRON MICROSCOPY

S.-M. Kim<sup>1</sup>, C.L. Pint<sup>2</sup>, P.B. Amama<sup>3,4</sup>, R.H. Hauge<sup>5</sup>, B. Maruyama<sup>3</sup>, <u>E.A. Stach<sup>1,6</sup></u>

<sup>1</sup>School of Materials Engineering and Birck Nanotechnology Center, Purdue

University, West Lafayette, IN, <sup>2</sup>Department of Physics and Astronomy, and Richard

E. Smalley Institute for Nanoscale Science and Technology, Rice University,

Houston, Texas, <sup>3</sup>Air Force Research Laboratory, Materials and Manufacturing

Directorate, Wright-Patterson Air Force Base, Ohio, and University of Dayton

Research Institute (UDRI), <sup>4</sup>University of Dayton, Dayton, Ohio, <sup>5</sup>Department of

Chemistry and Richard E. Smalley Institute for Nanoscale Science and Technology,

Rice University, Houston, Texas, <sup>6</sup>Center for Functional Nanomaterials, Brookhaven

National Laboratory, Upton, NY, USA

Break: 11<sup>00</sup>-11<sup>30</sup>

## THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

## 11<sup>30</sup>-12<sup>00</sup> HIGH-K, HIGH-Q MICROWAVE DIELECTRICS: WHAT IS THE COMPROMISE TODAY?

D. Suvorov, B. Jančar

Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia

#### 12<sup>00</sup>-12<sup>30</sup> KINETICS OF HIGH-TEMPERATURE SPREADING

E. Saiz<sup>1</sup>, A.P. Tomsia<sup>2</sup>

<sup>1</sup>Centre for Advanced Structural Ceramics, Department of Materials, Imperial College of London, UK, <sup>2</sup>Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

## 12<sup>30</sup>-13<sup>00</sup> MATERIALS TRANSPORT AND CRYSTALLIZATION DURING THE AI INDUCED LAYER EXCHANGE (ALILE) PROCESS

E. Spiecker<sup>1</sup>, B. Birajdar<sup>1</sup>, T. Antesberger<sup>2</sup>, M. Stutzmann<sup>2</sup>

<sup>1</sup>Center for Nanoanalysis and Electron Microscopy (CENEM), Materials Science and Engineering Department VII, University of Erlangen-Nürnberg, Erlangen, Germany, <sup>2</sup>Walter Schottky Institut and Physics Department, Technische Universität München, Garching, Germany

## 13<sup>00</sup>-13<sup>30</sup> NUCLEATION AND GROWTH OF COLLOIDAL NANOPARTICLES STUDIED BY COUPLED IN-SITU SPECTROSCOPIC METHODS

R. Kraehnert

Technical University of Berlin, Department of Chemistry, Berlin, Germany

Break: 13<sup>30</sup>-15<sup>00</sup>

#### SYMPOSIUM C: NANOSTRUCTURED MATERIALS

Tuesday, September 6, 2011

**Session I:** 15<sup>00</sup>-19<sup>00</sup>

Chairmen: M. Damnjanović and V. Uskoković

Conference Hall

15<sup>00</sup>-15<sup>15</sup> STRUCTURE, MAGNETISM AND ELECTRONIC PROPERTIES OF NANOCRYSTALLINE 3d-METALS ENCAPSULATED IN CARBON

A.Ye. Yermakov<sup>1</sup>, M.A. Uimin<sup>1</sup>, A.A. Mysik<sup>1</sup>, I.V. Byzov<sup>1</sup>, V.A. Tzurin<sup>1</sup>, Yu.S. Ponosov<sup>1</sup>, V.R. Galakhov<sup>1</sup>, E.Z. Kurmaev<sup>1</sup>, N.N. Schegoleva<sup>1</sup>, E.S. Lokteva<sup>2</sup>, A.V. Erokhin<sup>2</sup>, V.V. Lunin<sup>2</sup>

Institute of Metal Physics, Ural Branch of RAS, Ekaterinburg, Russia

Moscow State University. Chemical Department, Moscow, Russia

## 15<sup>15</sup>-15<sup>30</sup> SILICON NANOWIRE COATED MICROPARTICLES AS ADHESIVE DRUG DELIVERY DEVICES

V. Uskoković, T. Desai

Therapeutic Micro and Nanotechnology Laboratory, Department of Bioengineering and Therapeutic Sciences, University of California, San Francisco, USA

15<sup>30</sup>-15<sup>45</sup> A HIGH-TEMPERATURE OPTIAL STUDY OF DEFECTS AND DIFFUSION IN LITHIUM DEFICIENT LITHIUM NIOBATE

K.-D. Becker, J. Shi

Institute of Physical and Theoretical Chemistry, Technische Universität Braunschweig, Braunschweig, Germany

- 15<sup>45</sup>-16<sup>00</sup> (IN)COMMENSURABILITY OF CARBON NANOTUBES

  <u>M. Damnjanović</u>, I. Milošević

  NanoLab, Faculty of Physics, University of Belgrade, Belgrade, Serbia
- 16<sup>00</sup>-16<sup>15</sup> **PROPERTIES OF HELICALLY COILED NANOTUBES**<a href="I.Milošević">I.Milošević</a>, Z. Popović</a>, S. Dmitović</a>, M. Damnjanović
  <a href="NanoLab">NanoLab</a>, Faculty of Physics, University of Belgrade, Belgrade, Serbia
- 16<sup>15</sup>-16<sup>30</sup> THE PUZZLE-INTERLAYER MODEL: A UNIVERSAL APPROACH IN MATERIALS SCIENCE FOR DESCRIBING POROUS MATERIALS
  W. Gille
  Martin-Luther-University Halle-Wittenberg, Institute of Physics, Halle, Germany

## $16^{30}\text{--}16^{45}$ $\,$ MODEL OF "IN-SITU TENSILE TEST IN SEM" OF Al-Al\_4C\_3 $\,$ NANOMATERIALS

M. Besterci<sup>1</sup>, O. Velgosová<sup>2</sup>, J. Ivan<sup>3</sup>, B. Balloková<sup>1</sup>, K. Sülleiová<sup>1</sup>

Institute of Materials Research, Slovak Academy of Sciences, Košice, Slovak Republic, <sup>2</sup>Dept. of Non-ferrous Metals and Waste Treatment, Faculty of Metallurgy, Technical University, Košice, Slovak Republic, <sup>3</sup>Institute of Materials and Machine Mechanics, Slovak Academy of Sciences, Bratislava, Slovak Republic

# 16<sup>45</sup>-17<sup>00</sup> SOLVOTHERMAL SYNTHESIS OF NEW 2D LAYERED NANOCRYSTALLINE INORGANIC-ORGANIC HYBRID V<sub>4</sub>O<sub>4</sub>(OH)<sub>2</sub>(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>)·DMF COMPOUND AND ITS MAGNETIC PROPERTIES

<u>I. Djerdj</u><sup>1</sup>, Z. Crnjak Orel<sup>2</sup>, S.D. Škapin<sup>3</sup>, M. Čeh<sup>3</sup>, Z. Jagličić<sup>4,5</sup>, D. Pajić<sup>4,6</sup>, B. Kozlevčar<sup>7</sup>, Ž.K. Jaćimović<sup>8</sup>

<sup>1</sup>Ruđer Bošković Institute, Zagreb, Croatia, <sup>2</sup>National Institute of Chemistry, Ljubljana, Slovenia, <sup>3</sup>Institute Jožef Stefan, Ljubljana, Slovenia, <sup>4</sup>Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia, <sup>5</sup>Faculty of Civil and Geodetic Engineering, University of Ljubljana, Ljubljana, Slovenia, <sup>6</sup>Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia, <sup>7</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia, <sup>8</sup>Faculty of Metallurgy and Technology, Podgorica, Montenegro

Break: 17<sup>00</sup>-17<sup>30</sup>

## 17<sup>30</sup>-17<sup>45</sup> COMPOSITION – PROPERTIES RELATIONSHIP OF NANOSTRUCTURED POLYCARBONATE-BASED POLYURETHANE/ NANOCOMPOSITES

<u>R. Poręba<sup>1</sup></u>, M. Špírková<sup>1</sup>, J. Pavličević<sup>1</sup>, N. Lazić<sup>2</sup>

<sup>1</sup>Institute of Macromolecular Chemistry AS CR, v.v.i., Prague, Czech Republic <sup>2</sup>Institute of General and Physical Chemistry, Belgrade, Serbia

## 17<sup>45</sup>-18<sup>00</sup> FEATURES OF THE NANOSTRUCTURED MATERIALS FOR NONLINEAR OPTICS AND SOLAR ENERGY APPLICATIONS

N.V. Kamanina<sup>1</sup>, N.N. Rozhkova<sup>2</sup>, V.E. Vaganov<sup>3</sup>, D.P. Uskokovic<sup>4</sup>

<sup>1</sup>Vavilov State Optical Institute, St. Petersburg, Russia, <sup>2</sup>Institute of Geology Karelian Research Centre Russian Academy of Sciences, Petrozavodsk, Russia, <sup>3</sup>Vladimir State University (VlSU), Vladimir, Russia, <sup>4</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia

## 18<sup>00</sup>-18<sup>15</sup> PREPARATION OF METAL NANOPARTICLES FOR SOFC ANODES USING SONOELECTROCHEMICAL METHODS

P. Thanou<sup>1</sup>, P. Sakkas<sup>1</sup>, G. Sourkouni<sup>3</sup>, O. Schneider<sup>1,4</sup>, Chr. Argirusis<sup>1</sup>

National Technical University of Athens, School of Chemcial Engineering,
Zografou, Greece, <sup>2</sup>Clausthal University of Technology, Institute of Metallurgy,
Clausthal-Zellerfeld, Germany, <sup>3</sup>Clausthal University of Technology, Energy
Research Centre Lower Saxony, Goslar, Germany, <sup>4</sup>Technische Universität
München, Department of Physics, Chair for Energy Conversion and Storage,
Garching, Germany

# 18<sup>15</sup>-18<sup>30</sup> SINTERABILITY EVALUATION OF ALUMINUM METAL MATRIX COMPOSITES POWDER WITH DIFFERENT CHEMICAL COMPOSTITIONS

H. Rudianto<sup>1,2</sup>, S.-S. Yang<sup>1</sup>, Y.-J. Kim<sup>1</sup>, K.-W. Nam<sup>2</sup>

Powder technology Research Group, Korea Institute of Materials Science, Changwon, South Korea, <sup>2</sup>Department of UR Interdisciplinary Program of Mechanical Engineering, Pukyong National University, Busan, South Korea

# 18<sup>30</sup>-18<sup>45</sup> **DISPERSION STATE, OPTICAL CHARACTERIZATION AND ELECTRICAL PROPERTIES OF CARBON NANOTUBE / POLYMER COMPOSITES**

A. Combessis<sup>1,2</sup>, L. Flandin<sup>1</sup>, L. Bayon<sup>2</sup>, C. Mazel<sup>2</sup>

<sup>1</sup>LEPMI/LMOPS, Le Bourget du Lac, France, <sup>2</sup>NEXANS Research Center, Lyon, France

#### 18<sup>45</sup>-19<sup>00</sup> REACTIVITY OF NANOCRYSTALLINE MAGNESIUM

<u>I. Konstanchuk</u><sup>1</sup>, K. Gerasimov<sup>1</sup>, A. Demkin<sup>1</sup>, J.-L. Bobet<sup>2</sup>

<sup>1</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russian Federation, <sup>2</sup>Institut de Chimie de la Matière Condensée de Bordeaux ICMCB-CNRS, Université Bordeaux 1, Bordeaux, France

#### SYMPOSIUM C: NANOSTRUCTURED MATERIALS

Tuesday, September 6, 2011

**Session II:** 15<sup>00</sup>-18<sup>30</sup>

Chairmen: A. Ermakov and M.B. Plavšić

Small Hall

## 15<sup>00</sup>-15<sup>15</sup> **3D NANOSTRUCTURED OXIDES MATERIALS GROWN AT THE SURFACE OF LIQUID METALLIC ALLOYS**

A.N. Khodan

National Research Center "Kurchatov Institute", Moscow, Russian Federation

## 15<sup>15</sup>-15<sup>30</sup> STRUCTURE EVOLUTION AT HEATING OF FINEMET TYPE AMORPHOUS MICROWIRES

S.D. Kaloshkin<sup>1</sup>, M.N. Churyukanova<sup>1</sup>, <u>V.V. Tcherdyntsev</u><sup>1</sup>, E.V. Medvedeva<sup>2</sup>, A.A. Aleev<sup>3</sup>, O.A. Korchuganova<sup>4</sup>, S.V. Rogozhkin<sup>3</sup>

<sup>1</sup>National University of Science and Technology «MISIS», Moscow, Russia, <sup>2</sup>Institute

of Electrophysics, Ural Branch RAS, Ekaterinburg, Russia, <sup>3</sup>SSC RF Institute for Theoretical and Experimental Physics, Moscow, Russia, <sup>4</sup>National Research Nuclear University «MEPhI», Moscow, Russia

# 15<sup>30</sup>-15<sup>45</sup> SYNTHESIS AND INVESTIGATIONS OF STRUCTURE AND ELECTROCHEMICAL PROPERTIES OF PtCr/ EBONEX CATALYSTS FOR PEM WATER ELECTROLYSIS

G. Borisov, A. Stoyanova, E. Lefterova, E. Slavcheva Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, Sofia, Bulgaria

## 15<sup>45</sup>-16<sup>00</sup> MORPHOLOGY OF COMPOSITE INORGANIC MATRIX CONTAINING ION-EXCHANGER NANOPARTICLES

Yu.S. Dzyazko<sup>1</sup>, Yu.M. Volfkovich<sup>2</sup>, V.E. Sosenkin<sup>2</sup>, N.F. Nikolskaya<sup>2</sup>

<sup>1</sup>V.I. Vernadskii Institute of General & Inorganic Chemistry, Kiev, Ukraine

<sup>2</sup>A.N. Frumkin Institute of Physical Chemistry & Electrochemistry, Moscow, RF

## 16<sup>00</sup>-16<sup>15</sup> SYNTHESIS OF NICKEL FERRITE NANOPARTICLES BY THE CRUCIBLE-FREE AEROSOL TECHNIQUE

Yu.G. Morozov, O.V.Belousova, M.V. Kuznetsov Institute of Structural Macrokinetics and Materials Science Russian Academy of Sciences, Chernogolovka, Moscow Region, Russia

## 16<sup>15</sup>-16<sup>30</sup> HYDROGEN STATE IN MECHANICALLY PREPARED Ti/B NANOCOMPOSITE

O.S. Morozova<sup>1</sup>, T.I. Khomenko<sup>1</sup>, A.V. Leonov<sup>2</sup>, E.Z. Kurmaev<sup>3</sup>, Ch. Borchers<sup>4</sup>, I. Prochazka<sup>5</sup>

<sup>1</sup>Semenov Institute of Chemical Physics RAS, Moscow, Russia, <sup>2</sup>Department of Chemistry, Lomonosov Moscow State University, Leninskie Gory, Moscow, Russia, <sup>3</sup>Institute of Metal Physics, RAS-Ural Division, Ekaterinburg, Russia, <sup>4</sup>Institute for Material Physics, University of Göttingen, Goettingen, Germany, <sup>5</sup>Faculty of Mathematics and Physics, Charles University in Prague, Praha 8, Czech Republic

## 16<sup>30</sup>-16<sup>45</sup> MECHANICAL PROPERTIES OF RARE-EARTH DOPED Si₃N₄ AND Si₃N₄/SiC CERAMICS

P. Tatarko<sup>1</sup>, <u>J. Dusza</u><sup>1</sup>, P. Sajgalík<sup>2</sup>

<sup>1</sup>Institute of Materials Research, SAS, Kosice, Slovak Republic

<sup>2</sup>Institute of Inorganic Chemistry, SAS, Bratislava 45, Slovak Republic

## 16<sup>45</sup>-17<sup>00</sup> CHEMISTRY AND MOCVD APPLICATIONS OF VOLATILE DIMETHYLGOLD(III) COMPOUNDS WITH (O,N,S)-DONOR LIGANDS

N.B. Morozova

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

Break: 1700-1730

## $17^{30}$ - $17^{45}$ MICROSTRUCTURAL DESIGN OF YBCO SINGLE-GRAIN BULK SUPERCONDUCTORS WITH CeO<sub>2</sub> ADDITION

P. Diko, K. Zmorayová, M. Šefčiková, V. Antal, D. Volochová, S. Piovarči, J. Kováč Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovak Republic

#### 17<sup>45</sup>-18<sup>00</sup> ADHESIVE CONTACT OF ROUGH ELASTIC SOLIDS

B. Galanov, <u>I. Valeeva</u>, S. Ivanov Institute for Problems of Materials Science, NASc of Ukraine, Kiev, Ukraine

## 18<sup>00</sup>-18<sup>15</sup> CATALYTIC EFFECTS OF NANO-SIZED TiC, TiN, Nb<sub>2</sub>O<sub>5</sub>, Cr<sub>2</sub>O<sub>3</sub> AND NiCl<sub>2</sub> ON THE HYDROGEN STORAGE PROPERTIES OF LiAlH<sub>4</sub>

R.-u. Din, L. Ping, Q. Xuanhui

State Key Laboratory for Advanced Metals and Materials, School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, China

## 18<sup>15</sup>-18<sup>30</sup> COMPLEX EFFECT OF NANOFILLER ON STRUCTURE AND PROPERTIES OF POLYMER-MODIFIED EPOXY

#### I. Kelnar, J. Rotrekl

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

#### THIRD PLENARY SESSION

Wednesday, September 7, 2011

**Session III:** 09<sup>00</sup>-13<sup>00</sup>

Chairmen: R. Hull, J. Wittig and W. Jaeger

## 09<sup>00</sup>-09<sup>30</sup> ASSEMBLY OF HIERARCHICALLY SCALED SEMICONDUCTOR NANOSTRUCTURES

R. Hull

Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, USA

## 09<sup>30</sup>-10<sup>00</sup> INTERFACE AND DEFECT PHENOMENA OF SEMICONDUCTOR OXIDE NANOSTRUCTURES

Y. Ortega<sup>1,2</sup>, D. Maestre<sup>1,2</sup>, Ch. Dieker<sup>1</sup>, D. Häussler<sup>1</sup>, A. Cremades<sup>2</sup>, P. Fernández<sup>2</sup>, J. Pigueras<sup>2</sup>, W. Jaeger<sup>1</sup>

<sup>1</sup>Institute of Materials Science, Christian-Albrechts-University of Kiel, Kiel, Germany EU, <sup>2</sup> Dept. Materials Physics, University Complutense of Madrid, Madrid, Spain EU

# 10<sup>00</sup>-10<sup>30</sup> EXPLORING THE ARCHITECTURE OF SOLID SOLUTIONS WITH ATOM PROBE MICROSCOPY: A PATHWAY TOWARDS REMARKABLE NEW MATERIALS PROPERTIES

S.P. Ringer

Australian Centre for Microscopy & Microanalysis, The University of Sydney, NSW, Australia

Break: 10<sup>30</sup>-11<sup>00</sup>

#### 11<sup>00</sup>-11<sup>30</sup> THE FUTURE OF MAGNETIC DATA STORAGE

J. Wittig

Vanderbilt University, Nashville, Tennessee, USA

## 11<sup>30</sup>-12<sup>00</sup> SIZE-DEPENDENT MAGNETIC PROPERTIES OF SINGLE IRON-BASED NANOPARTICLES PROBED BY X-RAY SPECTROMICROSCOPY

A. Fraile Rodríguez<sup>1</sup>, A. Kleibert<sup>2</sup>, A. Balan<sup>2</sup>, J. Bansmann<sup>3</sup>, F. Nolting<sup>2</sup>, A. Romero<sup>1</sup>, C. Moya<sup>1</sup>, N. Pérez<sup>1</sup>, A. Labarta<sup>1</sup>, X. Batlle

<sup>1</sup>Dept de Física Fonamental and Institut de Nanociència i Nanotecnologia (IN2UB), Universitat de Barcelona, Barcelona, Spain, <sup>2</sup>Paul Scherrer Institut, Villigen PSI, Switzerland, <sup>3</sup>Institute of Surface Chemistry and Catalysis, University of Ulm, Ulm, Germany

## $12^{00}$ - $12^{30}$ MAGNETISM AND MAGNETIC MATERIALS FOR NONVOLATILE MEMORY

K.-H. Shin

KIST (Korea Institute of Science and Technology), Seoul, Korea

#### 12<sup>30</sup>-13<sup>00</sup> TOROIDAL METAMATERIALS

V.A. Fedotov, N.I. Zheludev

Optoelectronics Research Centre and Centre for Photonic Metamaterials, University of Southampton, UK

## THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

Herceg Novi, September 5-9, 2011

#### FORTH PLENARY SESSION

Thursday, September 8, 2011

Session IV: 09<sup>00</sup>-12<sup>30</sup>

Chairmen: S. Miloniić, R.A. Andrievski and K.-H. Shin

#### 09<sup>00</sup>-09<sup>30</sup> BEHAVIOR OF RADIATION EFFECTS IN NANOMATERIALS

R.A. Andrievski

Institute of Problems of Chemical Physics, Chernogolovka, Russia

## 09<sup>30</sup>-10<sup>00</sup> SYNTHESIS AND PHOTOCATALYTIC CHARACTERISTICS OF CARBON-TIO<sub>2</sub> HYBRID NANOWIRES AND NANOBELTS

E.-T. Kim

Department of Materials Science & Engineering, Chungnam National University, Daejeon, Republic of Korea

# 10<sup>00</sup>-10<sup>30</sup> THE REVOLUTIONARY RTILs - ROOM TEMPERATURE IONIC LIQUIDS AT ELECTRIFIED INTERFACES: FROM UNDERSTANDING TO APPLICATIONS

A.A. Kornvshev

Department of Chemistry, Faculty of Natural Sciences, Imperial College London, London, United Kingdom

## $10^{30}\text{-}11^{00}$ SILVER AND ALUMINUM BASE NANOCOMPOSITES PREPARED FROM BALL MILLED POWDERS

<u>J. Dutkiewicz</u>, L. Lityńska-Dobrzyńska, W. Maziarz, A. Kukuła Institute of Metallurgy and Materials Science of the Polish Academy of Sciences, Krakow, Poland

Break: 1100-1130

#### 11<sup>30</sup>-12<sup>00</sup> MICROBIAL ASPECTS IN CORROSION STUDIES

- FEMS Lecturer Award for Excellence in MSE 2010 -
- J. Michalska

Department of Materials Science, Silesian University of Technology, Katowice, Poland

## 12<sup>00</sup>-12<sup>30</sup> AFM-RAMAN-SNOM AND TIP ENHANCED RAMAN STUDIES OF MODERN NANOSTRUCTURES

P. Dorozhkin, A. Shchokin, E. Kuznetsov, V. Bykov, <u>I. Bykov</u> *NT-MDT Co., Zelenograd, Moscow, Russia* 

#### **SYMPOSIUM E: BIOMATERIALS**

Friday, September 9, 2011

**Session I:** 09<sup>00</sup>-11<sup>00</sup>

Chairmen: Dj. Koruga and N. Ignjatović

- 09<sup>00</sup>-09<sup>15</sup> MECHANOCHEMICAL SYNTHESIS AND CHARACTERIZATION OF II-VI NANOCRYSTALS: CHALLENGE FOR CYTOTOXICITY ISSUES

  P. Baláž<sup>1</sup>, R. Jardin<sup>2</sup>, G. Mojžišová<sup>3</sup>, J. Mojžiš<sup>3</sup>, E. Dutková<sup>1</sup>, M.J. Saygués<sup>4</sup>, E. Turianicová<sup>1</sup>, M. Baláž<sup>1</sup>

  Institute of Geotechnics, Slovak Academy of Sciences, Košice, Slovakia, <sup>2</sup>Bruker AXS GmbH, Karlsruhe, Germany, <sup>3</sup>P. J. Šafárik University, Faculty of Medicine, Košice, Slovakia, <sup>4</sup>Institute of Materials Science of Seville, Sevilla, Spain
- 09<sup>15</sup>-09<sup>30</sup> MEMBRANE BIOREACTOR BIOFOULING AS EXTRACELLULAR MATRIX: AN INNOVATIVE STRATEGY FOR MATERIALS DESIGN M. Herrera-Robledo, A. Noyola, V. Torres, V.M. Castano Environmental Nanotechnology group (NiA), National University of Mexico-Autonomous University of Queretaro (UNAM-UAQ), Mexico
- 09<sup>30</sup>-09<sup>45</sup> MULTIFUNCTIONAL NANO PARTICULATE SYSTEMS BASED ON HYDROXYAPATITE AS SYSTEMS FOR LOCAL DELIVERY OF VITAMIN D3

N. Ignjatović<sup>1</sup>, Z. Ajduković<sup>2</sup>, S. Drmanić<sup>3</sup>, D. Uskoković<sup>1</sup>

Institute of Technical Sciences of the SASA, Belgrade, Serbia, <sup>2</sup>Faculty of Medicine, Clinic of Stomatology, Department of Prosthodontics, Niš, Serbia, <sup>3</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

09<sup>45</sup>-10<sup>00</sup> ANTIBACTERIAL ACTIVITY AND CYTOTOXICITY OF HYDROXYAPATITE/SILVER NANOCOMPOSITES SYNTHESIZED BY A SONOCHEMICAL APPROACH

M. Vukomanović<sup>1,2</sup>, U. Repnik<sup>3</sup>, S. D. Škapin<sup>1</sup>, D. Uskoković<sup>2</sup>, D. Suvorov<sup>1</sup>

Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia,

Institute of Technical Sciences of SASA, Belgrade, Serbia, Department of Biochemistry, Molecular and Structural Biology, Jožef Stefan Institute, Ljubljana, Slovenia

## 10<sup>00</sup>-10<sup>15</sup> NONINVASIVE OPTICAL SENSING OF GLUCOSE IN WATER SOLUTION, BLOOD, AND HUMAN TISSUES

I. Koruga<sup>1</sup>, J. Munćan<sup>2</sup>, J. Šakota<sup>2</sup>, N. Jagodić<sup>3</sup>, <u>Dj. Koruga<sup>2</sup></u>

<sup>1</sup>DIA Systems, Inc., Fremont, CA 94538, USA, <sup>2</sup>NanoLab, Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Serbia, <sup>3</sup>Optix, Zemun, Serbia

# 10<sup>15</sup>-10<sup>30</sup> **FORCE MEASUREMENTS ON TEETH**J. Ferčec<sup>1</sup>, B. Glišič<sup>2</sup>, I. Šćepan<sup>2</sup>, E. Marković<sup>2</sup>, D. Stamenković<sup>2</sup>, I. Anžel<sup>1</sup>, <u>R. Rudol</u>f<sup>1,3</sup>

<sup>1</sup>University of Maribor, Faculty of Mechanical Engineering, Slovenia, <sup>2</sup>University of Belgrade, High School of Dentistry, Serbia, <sup>3</sup>Zlatarna Celje d.d., Slovenia

## $10^{30}$ - $10^{45}$ TECHNOLOGY OF PRODUCTION OF ANTIOXIDANTS PREPARATIONS FROM PLANT MATERIALS

<u>I. Lomovskiy</u>, O. Lomovsky Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia

# 10<sup>45</sup>-11<sup>00</sup> **DESIGNING MOLDS FOR RAPID ROTATIONAL FOAM MOLDING OF INTEGRAL-SKIN CELLULAR POLYOLEFIN COMPOSITES**R. Pop-Iliev

Faculty of Engineering and Applied Science, University of Ontario Institute of Technology, Oshawa, Ontario, Canada

#### 11<sup>00</sup>-11<sup>30</sup> CLOSING CEREMONY

#### POSTER SESSION I

Tuesday, September 6, 2011, 20<sup>30</sup>-22<sup>00</sup>

## SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

#### P.S.A.1. NANOCOMPOSITES OBTAINED BY HIGH PRESSURE TORSION POWDER CONSOLIDATION

A. Bachmaier, R. Pippan

Erich Schmid Institute, Austrian Academy of Sciences, Leoben, Austria

#### P.S.A.2. THE ISOELECTRIC POINT OF ZIRCONIA

J.J. Gulicovski, <u>S.K. Milonjić</u>
The Vinča Institute of Nuclear Sciences, Belgrade, Serbia

#### P.S.A.3. HYDROTHERMAL SYNTHESIS OF ZIRCONIUM SUBSTITUTED HYDROXYAPATITE

Z. Stojanović, M. Lukić, Lj. Veselinović, S. Marković, D. Uskoković Institute of Technical Sciences of SASA, Belgrade, Serbia

#### P.S.A.4. COLD PLASMA TREATMENT OF POLYMERIC MATRIX COMPOSITES

S. Guzmán, F. Velasco, N. Encinas, A. Bautista

Department of Materials Science and Engineering and Chemical Engineering,

Universidad Carlos III de Madrid, Leganés, Spain

## P.S.A.5. MECHANICAL MILLING PROCESS OF A PETROLEUM COKE WITH BORIC ACID FOR LITHIUM-ION BATTERIES

S. Guzmán<sup>1</sup>, F. Velasco<sup>1</sup>, M.E. Rabanal<sup>1</sup>, J.M. Jiménez-Mateos<sup>2</sup>

<sup>1</sup>Universidad Carlos III de Madrid, Materials Sci and Eng and Chemical Eng Dept, Leganés, Spain, <sup>2</sup>Repsol. Technology Dept. Ctra Nacional V, Móstoles, Spain

## P.S.A.6. EFFECT OF PLASMA MODIFICATION ON SURFACE PROPERTIES AND CHEMICAL STRUCTURE OF CHITOSAN/GELATIN/PLLA FILMS

<u>T. Demina<sup>1</sup></u>, D. Zaytseva-Zotova<sup>2</sup>, M. Yablokov<sup>1</sup>, A. Gilman<sup>1</sup>, T. Akopova<sup>1</sup>, E. Markvicheva<sup>2</sup>, A. Zelenetskii<sup>1</sup>

<sup>1</sup>Enikolopov Institute of Synthetic Polymer Materials, Russian Academy of Sciences, Moscow, Russia, <sup>2</sup>Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, Russia

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#### P.S.A.7. THE POSSIBILTIES OF THE MECHANOCHEMICAL MODIFICATION OF MoO<sub>3</sub>

N. Lytvyn<sup>1</sup>, V. Zazhigalov<sup>1</sup>, <u>K. Wieczorek-Ciurowa</u><sup>2</sup>

<sup>1</sup>Institute for Sorption and Problems of Endoecology, National Academy of Sciences of Ukraine, Kiev, Ukraine, <sup>2</sup>Faculty of Chemical Engineering and Technology, Cracow University of Technology, Cracow, Poland

#### P.S.A.8. RHEOLOGICAL PROPERTIES OF BIOPOLYMER MEMBRANS AND FRICTION EFFECTS

M.B. Plavšić, I. Pajić-Lijaković, M.M. Plavšić, B. Bugarski Faculty of Technology and Metallurgy, Belgrade University, Belgrade, Serbia

#### P.S.A.9. LOCAL DENSITY EFFECTS OF POLYMER NANO-STRUCTURED FILLER COMPOSITES

M.B. Plavšić<sup>1</sup>, N. Lazić<sup>2</sup>, I. Pajić-Lijaković<sup>1</sup> M.M. Plavšić<sup>1</sup>

Faculty of Technology and Metallurgy, Belgrade University, Belgrade, Serbia,

Institute for General and Physical Chemistry, Belgrade, Serbia

#### P.S.A.10. MICROSTRUCTURE AND PROPERTIES OF LaCoO<sub>3</sub> PEROVSKITE THIN FILMS DEPOSITED BY LASER ABLATION PROCESS

L. Cieniek

AGH – University of Science and Technology, Krakow, Poland

## P.S.A.11. SYNTHESIS AND CHARACTERIZATION OF LiM<sub>x</sub>Mn<sub>2-x</sub>O<sub>4</sub> CATHODE MATERIAL USING STARCH COMBUSTION METHOD

<u>I. Stojković</u><sup>1</sup>, M. Vujković<sup>1</sup>, N. Cvjetićanin<sup>1</sup>, S. Mentus<sup>1,2</sup>

University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia,

<sup>2</sup>The Serbian Academy of Science and Arts, Belgrade, Serbia

## P.S.A.12. SURFACE CHARACTERISTICS OF CARBONIZED HEMP ACTIVATED WITH POTASSIUM HYDROXIDE

M. Vukčević<sup>1</sup>, A. Kalijadis<sup>2</sup>, B. Babić<sup>3</sup>, M. Radišić<sup>1</sup>, B. Pejić<sup>1</sup>, Z. Laušević<sup>2</sup>, M. Laušević<sup>1</sup>

<sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, <sup>2</sup>Laboratory of Physics, Vinca Institute of Nuclear Sciences, Belgrade, <sup>3</sup>Laboratory of Material Science, Vinca Institute of Nuclear Sciences, Belgrade, Serbia

# P.S.A.13. CHARACTERISTICS OF THE THERMAL OXIDATION OF THIN POLYSILICON FILMS GROWN BY LPCVD AND HEAVILY IN SITU BORON-DOPED

S. Merabet<sup>1</sup>, M. Boukezzata<sup>2</sup>, H. Bouridah<sup>1</sup>, D. Bielle-Daspet<sup>3</sup>, G. Sarrabayrouse<sup>3</sup>

<sup>1</sup>Electronic Department, Faculty of Science Engineering, University of Jijel, Jijel, Algeria, <sup>2</sup>Electronic Department, Faculty of Science Engineering, University of Mentouri, Constantine, Algeria, <sup>3</sup>LAAS du CNRS, Toulouse cedex 4, France

#### P.S.A.14. INFLUENCE OF ATTRITION MILLING ON BARIUM TITANATE PROPERTIES

M.M. Vijatović Petrović<sup>1</sup>, <u>J.D. Bobić</u><sup>1</sup>, B.D. Stojanović<sup>1</sup>, S. Greičius<sup>2</sup>, P. Bowen<sup>3</sup>

<sup>1</sup>Institute for Multidisciplinary Research, Belgrade, Serbia, <sup>2</sup>Faculty of Physics, Vilnius University, Vilnius, Lithuania, <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

#### P.S.A.15. MECHANOCHEMICAL ACTIVATION OF THE REACTION BETWEEN SILICA AND CATECHOL

E.G. Shapolova<sup>1,2</sup>, O.I. Lomovsky<sup>1</sup>

<sup>1</sup>Institute of Solid State Chemistry and Mechanochemistry, Russian Academy of Sciences, Novosibirsk, Russia, <sup>2</sup>Research and Education Center "Molecular Design and Ecologically Safe Technologies", Novosibirsk State University, Novosibirsk, Russia

#### P.S.A.16. MAGNETORESISTANCE EFFECTS IN FERROMAGNETIC CHALCOPYRITE SEMICONDUCTORS

W. Dobrowolski<sup>1</sup>, L. Kilanski<sup>1</sup>, I. V. Fedorchenko<sup>2</sup>, S. A. Varnavskiy<sup>2</sup>, S. F. Marenkin<sup>2</sup>, D. K. Maude<sup>3</sup>

<sup>1</sup>Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, <sup>2</sup>Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia, <sup>3</sup>Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble, France

# P.S.A.17. PREPARATION AND CHARACTERIZATION OF NANO FERRITES Z.Ž. Lazarević<sup>1</sup>, Č. Jovalekić<sup>2</sup>, A. Milutinović<sup>1</sup>, M.J. Romčević<sup>1</sup>, N.Ž. Romčević<sup>1</sup> Institute of Physics, University of Belgrade, Zemun, Belgrade, Serbia, <sup>2</sup>The Institute for Multidisciplinary Research, Belgrade, Serbia

# P.S.A.18. THE INFLUENCE OF THE DETONATION SPRAYING PARAMETERS ON THE PHASE COMPOSITION AND MICROSTRUCTURE OF TiO<sub>2</sub>-Ag COATINGS

 $\text{D.V. Dudina}^1, \underline{\text{A.L. Bychkov}}^1, \text{S.B. Zlobin}^2, \text{V.Yu. Ulianitsky}^2, \text{N.V. Bulina}^1, \text{O.I. Lomovsky}^1$ 

<sup>1</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk Russia; <sup>2</sup>Lavrentiev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia

## P.S.A.19. SYNTHESIS AND STRUCTURE OF COPPER(II) COMPLEX WITH PYRIDOXALAMINOGUANIDINE AND O-PHENANTROLINE

M.M. Lalović, V.M. Leovac, Lj.S. Vojinović-Ješić, V.I. Češljević Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, Novi Sad, Serbia

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#### P.S.A.20. STRUCTURE AND PROPERTIES ZIRCONIA AND THEIR EVOLUTION AFTER LOW TEMPERATURE ANNEALING

E.V. Klevtsova, S.N. Kulkov

Institute of Strength Physics and Material Science SB RAS, Tomsk State University, Tomsk. Russia.

#### P.S.A.21. THERMOGRAPHIC PROPERTIES OF EUROPIUM DOPED YTTRIUM-GADOLINIUM OXIDE NANOPHOSPHOR

M.G. Nikolić, Ž. Antić, R.M. Krsmanović, V. Djordjević, T. Dramićanin, M.D. Dramićanin

Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

#### P.S.A.22. INFLUENCE OF MECHANICAL ACTIVATION ON THE ELECTRICAL AND MAGNETIC PROPERTIES OF FERRITE POWDERS

Z. Ristanović, M. Dobričić, D. Brajović, D. Sretenović Technical College Čačak, Serbia

#### P.S.A.23. LINEAR AND NONLINEAR OPTICAL SPECTRA FOR INTERSUBBAND TRANSITIONS OF CORE/SHELL (CdSe/ZnS BASED) SPHERICAL **OUANTUM DOTS**

R. Kostić, D. Stojanović

University of Belgrade, Institute of Physics, Belgrade, Serbia

#### P.S.A.24. EFFECT OF ELECTRIC FIELD ON GROUND AND EXCITED STATES D<sup>0</sup> BINDING ENERGY IN CdTe/ZnTe SPHERICAL QUANTUM DOT

D. Stojanović, R. Kostić

University of Belgrade, Institute of Physics, Belgrade, Serbia

#### P.S.A.25. LAYERED CORE-SHELL MODEL FOR DELIVERING **NANOBIOMATERIALS**

S. Armaković<sup>1</sup>, A.J. Šetrajčić-Tomić<sup>2</sup>, Lj.D. Džambas<sup>3</sup>, J.P. Šetrajčić<sup>1</sup>,\*, S. Krnetić<sup>4</sup>, S.M. Vučenović<sup>5</sup>

<sup>1</sup>University of Novi Sad, Faculty of Sciences, Department of Physics, Vojvodina – Serbia, <sup>2</sup>University of Novi Sad, Medical Faculty, Department of Pharmacy, Vojvodina – Serbia, <sup>3</sup>University of Novi Sad, Medical Faculty, Department of Dentistry, Vojvodina – Serbia, <sup>4</sup>University of Banja Luka, Faculty of Sciences – Chemistry, Republic of Srpska – B&H, <sup>5</sup>University of Banja Luka, Faculty of Sciences – Physics, Republic of Srpska – B&H, \*Academy of Sciences and Arts of the Republic of Srpska – B&H

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#### P.S.A.26. ELECTROCHEMICAL PROPERTIES OF ANODICALLY GROWN TiO<sub>2</sub>

N. Cvjetićanin<sup>1</sup>, T. Barudžija<sup>2</sup>, <u>D. Jugović</u><sup>3</sup>, M. Mitrić<sup>2</sup>

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## P.S.A.27. INFLUENCE OF SIC NANOPARTICLES ON THE MECHANICAL PROPERTIES OF Si<sub>1</sub>N<sub>4</sub>-SiC COMPOSITES

M. Kašiarová<sup>1</sup>, J. Dusza<sup>1</sup>, M. Hnatko<sup>2</sup>, P. Šajgalík<sup>2</sup>

<sup>1</sup>Institute of Materials Research, Slovak Academy of Sciences, Košice, Slovak Republic; <sup>2</sup>Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovak Republic

#### P.S.A.28. THE INFLUENCE OF A FORCED FLOW ON DENDRITIC GROWTH IN BINARY MELTS

A.P. Malygin<sup>1</sup>, D.V. Alexandrov<sup>1</sup>, P.K. Galenko<sup>2,3</sup>

<sup>1</sup>Department of Mathematical Physics, Urals State University, Ekaterinburg, Russian Federation, <sup>2</sup>Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luftund Raumfahrt (DLR), Köln, Germany, <sup>3</sup>Institut für Festkörperphysik, Ruhr-Universität Bochum, Bochum, Germany

## P.S.A.29. RECENT ACHIEVEMENTS IN INVESTIGATIONS OF BAYER ALUMINUM TRIHYDROXIDE GROWTH

I. Nikolić, D. Blečić

Faculty of Metallurgy and Technology, University of Montenegro, Podgorica, Montenegro

#### P.S.A.30. CHEMICAL PRECIPITATION SYNTHESIS AND CHARACTERIZATION OF Zr-DOPED HYDROXYAPATITE NANOPOWDERS

M.J. Lukić<sup>1</sup>, A. Stanković<sup>1</sup>, Lj. Veselinović<sup>1</sup>, S. D. Škapin<sup>2</sup>, I. Bračko<sup>2</sup>, S. Marković<sup>1</sup>, D. Uskoković<sup>1</sup>

<sup>1</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>Jožef Stefan Institute, Ljubljana, Slovenia

#### P.S.A.31. CASTABILITY OF ALUMINIUM ALLOYS

B. Zlatičanin, I. Bošković

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#### P.S.A.32. ELABORATION OF POROUS INSULATING MATERIALS STARTING FROM ALGERIAN FIRECLAYS

K. Boumchedda<sup>1</sup>, A. Ayadi<sup>2</sup>, B. Ghernouti<sup>3</sup>

<sup>1</sup>UR-MPE, FSI, University of Boumerdes, Boumerdes Algeria, <sup>2</sup>UR-MPE, FSI, University of Boumerdes, Boumerdes Algeria, <sup>3</sup>UR-MPE, FSI, University of Mascara, Algéria

## P.S.A.33. THE COMPARATIVE PROPERTIES OF SINTERED PRODUCTS BASED ON CLAYS FROM THE MINE BAUXITE "BIJELE POLJANE"

M. Krgović<sup>1</sup>, I. Bošković<sup>1</sup>, M. Vukčević<sup>1</sup>, R. Zejak<sup>2</sup>, M. Knežević<sup>2</sup>, B. Zlatičanin<sup>1</sup> *University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>University of Montenegro, Faculty of Civil Engineering, Podgorica, Montenegro* 

# P.S.A.34. PREPARATION AND CHARACTERIZATION OF Pt NANOCATALYST ON TUNGSTEN BASED SUPPORT FOR ALKALINE FUEL CELLS APPLICATIONS

<u>Lj. Gajić-Krstajić</u>, N.R. Elezović<sup>2</sup>, B.M. Babić<sup>3</sup>, V.V. Radmilović<sup>4</sup>, N.V. Krstajić<sup>5</sup>, Lj.M. Vračar<sup>5</sup>

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## P.S.A.35. A STUDY ON THE HYDROGEN STORAGE CAPACITY OF Pd - PLATED POROUS ACTIVATED CARBON

S. Randjić<sup>1</sup>, L. Ribić-Zelenović<sup>2</sup>, A. Maričić<sup>1</sup>, M. Spasojević<sup>2</sup>

<sup>1</sup>Technical Faculty Čačak, University of Kragujevac, Serbia

<sup>2</sup>Faculty of Agronomy Čačak, University of Kragujevac, Serbia

# P.S.A.36. THE EFFECT OF STRUCTURAL CHANGES DURING HEATING OF THE Ni<sub>79</sub>Co<sub>18.6</sub>Cu<sub>2,3</sub>AMORPHOUS POWDER ON ELECTRICAL AND MAGNETIC PROPERTIES

M. Spasojević<sup>1</sup>, P. Mašković<sup>1</sup>, L. Ribić-Zelenović<sup>1</sup>, A. Maričić<sup>2</sup>

Faculty of Agronomy Čačak, University of Kragujevac, Serbia

Techical Faculty Čačak, University of Kragujevac, Serbia

## $P.S.A.37. \quad \textbf{MONITORING OF HYDROGEN ABSORPTION/DESORPTION INTO PRESSED Ni<sub>97,1</sub>Co<sub>18,6</sub>Cu<sub>2,3</sub> POWDER USING RESISTOMETRY}$

A. Maričić<sup>1</sup>, S.Djukić<sup>1</sup>, L.Ribić-Zelenović<sup>2</sup>, M.Spasojević<sup>2</sup>

<sup>1</sup>Technical Faculty Čačak, University of Kragujevac, Serbia

<sup>2</sup>Faculty of Agronomy Čačak, University of Kragujevac, Serbia

## P.S.A.38. PROPERTIES OF THE ELECTROCHEMICALLY OBTAINED Ni<sub>65</sub>Fe<sub>24</sub>W<sub>11</sub> ALLOY POWDER

<u>L. Ribić-Zelenović</u><sup>1</sup>, N. Ćirović<sup>2</sup>, M. Spasojević<sup>1</sup>, N. Mitrović<sup>2</sup>, A. Maričić<sup>2</sup>

<sup>1</sup>Faculty of Agronomy Čačak, University of Kragujevac, Serbia

<sup>2</sup>Techical Faculty Čačak, University of Kragujevac, Serbia

# P.S.A.39. KINETICS OF CRYSTALLIZATION AND PHASE TRANSFORMATION OF Fe<sub>75</sub>Ni<sub>2</sub>Si<sub>8</sub>B<sub>13</sub>C<sub>2</sub> AMORHOUS ALLOY

D.M. Minić, N. Filipović, <u>V.A. Blagojević</u> Faculty for Physical Chemistry, University of Belgrade, Serbia

# P.S.A.40. SYNTHESIS OF THE NANOSTRUCTURED YAP:Ce VIA SPRAY PYROLYSIS BY POLYMERIC PRECURSOR SOLUTION

<u>V. Lojpur<sup>1</sup></u>, L. Mančić<sup>1</sup>, Maria Eugenia Rabanal<sup>2</sup>, Olivera Milošević<sup>1</sup>

Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>University Carlos III of Madrid, Dept. of Material Science and Engineering and Chemical Engineering, Leganes, Madrid, Spain

## P.S.A.41. FORMATION OF SOLIDS FROM THE GAS MIXTURES OF CARBON, NITROGEN AND HYDROGEN AT HIGH TEMPERATURES

J. Radić-Perić

Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

# P.S.A.42. FORMATION OF γ-AITI INTERMETALLIC INDUCED BY LASER IRRADIATION OF AI/TI NANO-STRUCTURES

<u>D. Peruško</u><sup>1</sup>, S. Petrović<sup>1</sup>, Z. Siketić<sup>2,3</sup>, M. Mitrić<sup>1</sup>, M. Čizmović<sup>1</sup>, M. Obradović<sup>1</sup>, D. Pjević<sup>1</sup>, M. Milosavljević<sup>1</sup>

<sup>1</sup>VINČA Institute of Nuclear Sciences, Belgrade University, Belgrade, Serbia, <sup>2</sup>Jožef Stefan Institute, Ljubljana, Slovenia, <sup>3</sup>Rudjer Bošković Institute, Zagreb, Croatia

# P.S.A.43. SYNTHESIS AND CHARACTERIZATION OF Co(II,) Ni(II) AND Cu(II) COMPLEXES WITH 1-HYDRAZINOPHTHALAZINE BASED LIGAND

J. Magyari, <u>B. Holló</u>, V. Leovac, K. Mészáros Szécsényi, V. Divjaković *University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia* 

# P.S.A.44. CHANGES IN THE ELECTRONIC STRUCTURE DURING THE HYDROGEN-INDUCED LITHIUM AMIDE/IMIDE TRANSFORMATION

N. Ivanović<sup>1</sup>, I. Radisavljević<sup>1</sup>, N. Novaković<sup>1</sup>, B. Paskaš-Mamula<sup>1</sup>, D. Colognesi<sup>2</sup> Institute of Nuclear Sciences "VINČA", Belgrade, Serbia, <sup>2</sup>Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, esto Fiorentino (FI), Italy

# P.S.A.45. STRUCTURAL CHARACTERIZATION OF MECHANICALLY ACTIVATED MgO-TiO<sub>2</sub> SYSTEM

<u>S. Filipović</u><sup>1</sup>, N. Obradović<sup>1</sup>, J. Krstić<sup>2</sup>, D. Kosanović<sup>1</sup>, M. Šćepanović<sup>3</sup>, V. Pavlović<sup>1</sup>, A. Maričić<sup>4</sup>, M. M. Ristić<sup>5</sup>

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# P.S.A.46. EFFECT OF TEMPERATURE AND pH ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF COBALT FERRITE (CoFe<sub>2</sub>O<sub>4</sub>) NANOPARTICLES OBTAINED VIA THE HYDROTHERMAL METHOD S. Makević, M. Logar, D. Suvorov Jožef Stefan Institute, Advanced Materials Department, Ljubljana, Slovenia

# P.S.A.47. KINETICS OF DRUG RELEASE FROM HYDROXYAPATITE B. Čolović, V. Jokanović Institute for Nuclear Sciences "Vinča", Laboratory for radiation chemistry and physics, Belgrade, Serbia

# P.S.A.48. REMELTING OF M-CrAIY AIR PLASMA SPRAYED COATINGS BY MEANS OF ALUMINIUM COLD ROLLING AND CONVENTIONAL HEAT TREATMENT

L. Čelko<sup>1</sup>, V. Řičánková<sup>1</sup>, L. Klakurková<sup>1</sup>, K. Zábranský<sup>2</sup>, J. Švejcar<sup>1</sup>

Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic, <sup>2</sup>Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic

# P.S.A.49. FORMATION OF HYPEREUTECTIC ALUMINIUM ALLOY FROM SACRIFICIAL NICKEL COATING INVESTIGATED BY DIFFERENTIAL THERMAL AND MICROSTRUCTURAL ANALYSIS

L. Klakurková<sup>1</sup>, L. Čelko<sup>1</sup>, S. Zlá<sup>2</sup>, B. Smetana<sup>2</sup>

<sup>1</sup>Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic, <sup>2</sup>Department of Physical Chemistry and Theory of Technological Processes, Faculty of Metallurgy and Materials Engineering, VŠB-Technical University of Ostrava, Ostrava, Czech Republic

# P.S.A.50. PREPARATION OF PLATINUM ELECTROCATALYST BY HYDROGEN ION-BEAM IRRADIATION

Z. Jovanović<sup>1</sup>, I. Pašti<sup>3</sup>, A. Kalijadis<sup>1</sup>, M. Laušević<sup>2</sup>, Z. Laušević<sup>1</sup>

Vinča Institute of Nuclear Sciences, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

# P.S.A.51. RELATIONS BETWEEN J-, M- AND N- INTEGRALS AND THOSE WITH INTERACTIONS ENERGY IN A BRITTLE MATERIAL

M. Touati, M. Chabaat

Built Env. Research Lab, Department of Structures and Materials, Civil Engineering Faculty, University of Sciences and Technology Houari Boumediene B. P. 32 El-Alia, Bab Ezzouar, Algiers, Algeria

# P.S.A.52. SYNTHESIS OF PENTLANDITES WITH VARIABLE COMPOSITION AND PHASE TRANSFORMATIONS UPON HEATING IN INERT ATMOSPHERE AND AIR

R.I. Gulyaeva, E.N. Selivanov, A.D. Vershinin
Institute of Metallurgy, Ural Branch, Russian Academy of Sciences, Yekaterinburg,
Russia

#### POSTER SESSION II

Wednesday, September 7, 2011, 20<sup>30</sup>-22<sup>00</sup>

# SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

# P.S.B.1. MECHANISM OF PHOTOCATALYTIC DEGRADATION OF METOPROLOL IN AQUEOUS TITANIUM DIOXIDE SUSPENSION B. Abramović<sup>1</sup>, S. Kler<sup>1</sup>, D. Šojić<sup>1</sup>, M. Laušević<sup>2</sup>, T. Radović<sup>2</sup>, D. Vione<sup>3</sup> <sup>1</sup>Faculty of Sciences, Novi Sad, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>Dipartimento di Chimica Analitica, Torino, Italy

# P.S.B.2. GROWTH AND MAGNETIC PROPERTIES OF InSb-MnSb EUTECTIC COMPOSITION

<u>I.V. Fedorchenko<sup>1</sup></u>, V.M.Novotortsev<sup>1</sup>, S.F.Marenkin<sup>1</sup>, A.V. Kochura<sup>2</sup>, W.D. Dobrowolski<sup>3</sup>

<sup>1</sup>Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia, <sup>2</sup>South - West State University, Kursk, Russia, <sup>3</sup>Institute of Physics PAS, Warszaw, Poland

# P.S.B.3. ELECTRON STRUCTURE AND OPTICAL PROPERTICS OF $Gd_3Ga_5O_{12}$ GARNET DOPED WITH Tb

<u>I.D. Shcherba<sup>1,2</sup></u>, L. Kostyk<sup>2</sup>, D. Uskokovic<sup>3</sup>, O. Tsvetkova<sup>2</sup>, A. Stosyk<sup>2</sup>, B. Jatsyk<sup>4</sup>, R. Kokosza<sup>1</sup>

<sup>1</sup>Institute of Techniques, University of Pedagogy, Krakow, Poland, <sup>2</sup>Lviv National University by Ivan Franko, Lviv, Ukraine, <sup>3</sup>Institute of Technical Sciences, SASA, Belgrade, Serbia, <sup>4</sup>University of Forestry and Wood Technology, Lviv, Ukraine

# P.S.B.4. CRYSTAL GROWTH RATE IN Y<sub>1.5</sub>Ba<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub> WITH CeO<sub>2</sub> ADDITION <u>K. Zmorayová</u>, D. Volochová, M. Šefčiková, M. Kalmanová, S. Piovarči, P. Diko *Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia*

# $P.S.B.5. \quad \begin{array}{ll} \textbf{TEMPERATURE OF SELFNUCLEATION IN } Y_{1.5}Ba_2Cu_3O_x \ WITH \ CeO_2 \\ \textbf{ADDITION} \end{array}$

M. Šefčiková, M. Kalmanová, K. Zmorayová, D. Volochová, S. Piovarči, P. Diko *Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia* 

# P.S.B.6. OPTIMIZATION OF HEAT TREATMENT AND ITS INFLUENCE ON CORROSION BEHAVIOUR OF AZ61 MAGNESIUM ALLOY

P. Doležal<sup>1</sup>, B. Hadzima<sup>2</sup>, M. Horynová<sup>1</sup>, L. Bukovinová<sup>2</sup>

<sup>1</sup>Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic, <sup>2</sup>Department of Materials Engineering, Faculty of Mechanical Engineering, University of Žilina, Slovak Republic

# P.S.B.7. IMPACT ANALYSIS OF SHOT PEENING OF ALUMINIUM ALLOY AW 6082 ON THE FATIGUE PROPERTIES

V. Škorík¹, F. Nový¹, P. Doležal², B. Hadzima¹, M. Horynová²
¹Department of Materials Engineering, Faculty of Mechanical Engineering,
University of Žilina, Slovak Republic, ¹Institute of Materials Science and
Engineering, Faculty of Mechanical Engineering, Brno University of Technology,
Czech Republic

#### P.S.B.8. REAGENT OXIDATION OF INTERMETALLIDE NbAl<sub>3</sub>

A.G. Upolovnikova, L.Y. Udoeva, V.M. Chumarev
Institute of Metallurgy, Ural Division, Russian Academy of Sciences, Ekaterinburg,
Russia

#### P.S.B.9. MAGNETOCALORIC EFFECT IN NI-MN-GA BASED ALLOYS

K. Sielicki, R. Wroblewski, M. Leonowicz
Faculty of Materials Science and Engineering, Warsaw University of Technology,
Warsaw, Poland

# P.S.B.10. IMPEDANCE SPECTROSCOPY OF MULTIDOPED CERIA M. Stojmenović<sup>1</sup>, S. Bošković<sup>1</sup>, S. Zec<sup>1</sup>, B. Matović<sup>1</sup>, S. Mentus<sup>2</sup>

Institute of Nuclear Sciences "Vinča", Belgrade, Serbia,

Faculty of Phisical Chemistry, University of Belgrade, Belgrade, Serbia

# P.S.B.11. MONTE CARLO ANALYSIS OF THE INFLUENCE OF DIFFERENT PACKAGING ON MOSFET ENERGY RESPONSE TO X-RAY AND GAMMA RADIATION

S.J. Stanković<sup>1</sup>, R.D. Ilić<sup>1</sup>, B. Lončar<sup>2</sup>, K. Janković<sup>3</sup>, M. Živanović<sup>1</sup>

Vinča Institute of Nuclear Sciences, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia, <sup>3</sup>Institute for testing materials-IMS, Belgrade, Serbia

## P.S.B.12. THE TOUGHNESS AND FATIGUE ANALYSIS OF Nd-Fe-B/EPOXY MAGNETIC COMPOSITES

<u>A. Stajčić</u><sup>1</sup>, A. Grujić<sup>1</sup>, J. Stajić-Trošić<sup>1</sup>, M. Stijepović<sup>2,3</sup>, D. Nedeljković<sup>1</sup>, S. Putić<sup>3</sup>, P.S. Uskoković<sup>3</sup>

<sup>1</sup>Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Department of Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar, <sup>3</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia

# P.S.B.13. ELECTROCHEMICAL STUDY OF COMPLEX FORMATION BETWEEN SOME TRANSITION CATIONS AND N,N',N",TETRAKIS(2-PYRIDYLMETHYL)-1,4,8,11-TETRAAZACYCLOTETRADECANE

B.B. Petković<sup>1</sup>, S. Stevanović<sup>2</sup>, D. Stanković<sup>3</sup>, R. Micić<sup>1</sup>, M. Budimir<sup>1</sup>, S.P. Sovilj<sup>3</sup>, V.M. Jovanović<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Natural Sciences and Mathematics, University of Priština, Kosovska Mitrovica, Serbia, <sup>2</sup>ICTM, Department of Electrochemistry, Belgrade, Serbia, <sup>3</sup>Faculty of Chemistry, University of Belgrade, Belgrade, Serbia

# P.S.B.14. ANALYSIS OF TERMALLY ACTIVATED PROCESSES IN COLD ROLLED AND ANNEALED Ni<sub>3</sub>Al BASED INTERMETALLIC STRIPS

P. Jozwik, Z. Bojar, C. Senderowski

Military University of Technology, Department of Advanced Materials and Technologies, Warsaw, Poland

# P.S.B.15. THERMAL STABILITY OF FeAI SINTERS STRUCTURE WITH ADDITION OF Al<sub>2</sub>O<sub>3</sub> NANOMETRIC CERAMIC

T. Durejko, S. Lipinski, Z. Bojar

Military University of Technology, Department of Advanced Materials and Technologies, Warsaw, Poland

#### P.S.B.16. STRUCTURE CHANGES AT CRYSTALLIZATION OF Zr<sub>57</sub>Ta<sub>8</sub>Nb<sub>2.5</sub>Cu<sub>13.4</sub>Ni<sub>11.1</sub>Al<sub>7.5</sub> AMORPHOUS ALLOY

S. Mudry <sup>1</sup>, V. Prokhorenko<sup>2</sup>, S. Prokhorenko<sup>2</sup>, <u>Z. Bojar</u><sup>3</sup>, J. Bystrzycki<sup>3</sup>, A.J. Panas<sup>3</sup> <sup>1</sup>Ivan Franko Lviv National University, Lviv, Ukraine, <sup>2</sup>National University "Lvivska Politechnika", Lviv, Ukraine, <sup>3</sup>Military University of Technology, Warsaw, Poland

## P.S.B.17. FORMATION OF THE SOLID SOLUTION Cr<sub>0.9</sub>Ta<sub>0.1</sub>Si<sub>2</sub> IN THE COURSE OF SOLID PHASE INTERACTION

L.I. Ieremenko, I.V. Kud, L.S. Likhoded, D.P. Zyatkevich, I.V. Uvarova Frantsevych Institute for Problems of Materials Science of NAS of Ukraine, Kyiv, Ukraine

## P.S.B.18. MODELLING OF ELECTRONS AND HEAVY PARTICLES IN PURE H<sub>2</sub> DISCHARGE

V. Stojanović, <u>Ž. Nikitović</u>, Z. Lj. Petrović Institute of Physics University of Belgrade, Belgrade, Serbia

# P.S.B.19. TEMPERATURE AND PRESSURE DEPENDENCE OF RAMAN SPECTRA IN CRYSTALLINE GeS<sub>2</sub>, AND GeSe<sub>2</sub>

Z.M. Jakšić<sup>1</sup>, Lj. Budinski–Petković<sup>2</sup>, I. Lončarević<sup>2</sup>, S.B. Vrhovac<sup>1</sup>

Institute of Physics, Belgrade, Serbia, <sup>2</sup>Faculty of Engineering, Novi Sad, Serbia

# P.S.B.20. CHANGES IN MICROSTRUCTURE AND MECHANICAL PROPERTIES OF Ni-25%Mo-8%Cr ALLOY AFTER LONG TIME ANNEALING AT 650 °C

E. Stępniowska

AGH University of Science and Technology, Kraków, Poland

# P.S.B.21. THE DETERMINATION OF INERTIA MOMENTS OF DETAILS WITH COMPLEX SHAPE

A. Hajderi<sup>1</sup>, V. Kasemi<sup>2</sup>

<sup>1</sup>Department of Engineering Sciences, Professional Studies Faculty, "Aleksander Moisiu" University, Durres, Albania, <sup>2</sup>University "Ismail Qemali" of Vlora, Albania

# P.S.B.22. PECULIARITIES OF THE MoSi<sub>2</sub>-CrSi<sub>2</sub> SOLID SOLUTION FORMATION DEPENDING ON THE CONDITIONS OF SOLID PHASE SYNTHESIS

I. Kud, L. Likhoded, L. Yeremenko, D. Zyatkevich, I. Uvarova

Frantsevych Institute for Problems of Materials Science of NAS of Ukraine, Kyiv,

Ukraine

# P.S.B.23. INSTRUMENTED INDENTATION OF WC-Co CEMENTED CARBIDES <u>A. Duszová</u>, P. Horňák, P. Hvizdoš, F. Lofaj, J. Dusza Institute of Materials Research, SAS, Kosice, Slovakia

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## P.S.B.24. MICROSTRUCTURE AND MECHANICAL PROPERTIES OF FRICTION STIR WELDED OF A 7042 ALUMINIUM

M. Kopyściański

Faculty of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology, Kraków, Poland

# P.S.B.25. CORROSION RESISTANCE OF FRICTION STIR WELDED 7XXX SERIES ALUMINUM ALLOYS

I. Kalemba

AGH University of Science and Technology, Kraków, Poland

# P.S.B.26. STRUCTURE AND PROPERTIES OF Ti(C,N,O) THIN FILMS DEPOSITED BY PLD TECHNIQUE ON POLYURETHANE SUBSTRATE

S. Kac<sup>1</sup>, R. Major<sup>2</sup>

<sup>1</sup>AGH-University of Science and Technology, Faculty of Metals Science and Industrial Computer Science, Krakow, Poland, <sup>2</sup>Institute of Metallurgy and Materials Science of Polish Academy of Sciences, Krakow, Poland

# P.S.B.27. PROCESSING AND CHARACTERIZATION OF COMPOSITE POLY (METHYLMETHACRYLATE)-BISMUTH-SILICON-OXIDE

<u>I. Radović</u><sup>1</sup>, S. Musbah<sup>1</sup>, D. Stojanović<sup>1</sup>, M. Zrilić<sup>1</sup>, N. Romčević<sup>2</sup>, V. Radojević<sup>1</sup>, R. Aleksić<sup>1</sup>

<sup>1</sup>Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Institute of Physics, Zemun. Serbia

# P.S.B.28. ON-LINE AND OFF-LINE PYROLYSIS FOR DETERMINATION OF POLY(VINYLPYRROLIDONE) IN WASTEWATER SAMPLES

M. Antić¹, <u>B. Jovančićević</u>², V. Antić¹, A. Kronimus³, K. Oing³, J. Schwarzbauer³ Faculty of Agriculture, Zemun, Serbia; <sup>2</sup>Faculty of Chemistry, Belgrade, Serbia; <sup>3</sup>Institute of Geology and Geochemistry of Petroleum and Coal, RWTH Aachen University, Aachen, Germany

# P.S.B.29. LOW-CYCLE FATIGUE OF THERMALLY-CYCLED CARBON-EPOXY COMPOSITE

E.M. Gutman, Ya. Unigovski, A. Grinberg, R. Shneck Dept of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel

## P.S.B.30. TENSILE PROPERTIES OF NOVEL POLYCARBONATE-BASED POLYURETHANE ELASTOMERS

Z. Hrdlička<sup>1</sup>, A. Kuta<sup>1</sup>, R. Poręba<sup>2</sup>, M. Špírková<sup>2</sup>, J. Pavličević<sup>2</sup>

Department of Polymers, Institute of Chemical Technology, Prague, Czech Republic, <sup>2</sup>Nanostructured Polymers and Composites Department, Institute of Macromolecular Chemistry AS CR, v.v.i., Prague, Czech Republic

# P.S.B.31. INFLUENCE OF THERMAL TESTS ON PHASE TRANSFORMATION IN NANOSTRUCTURED CERAMICS ZrO<sub>2</sub>(MgO)

V.V. Promakhov<sup>1</sup>, S.P. Buyakova<sup>1,2</sup>, S.N. Kulkov<sup>1,2</sup>

Institute of Strength Physics and Materials Science, Tomsk, Russia

<sup>2</sup>Tomsk State University, Tomsk, Russia

## P.S.B.32. STRUCTURE AND PROPERTIES OF ZIRCONIA-ALUMINA CERAMICS BASED ON OXIDE-HYDROXIDE MIXTURES

A.V. Kozlova<sup>1</sup>, I.A. Zhukov<sup>1</sup>, S.P. Buyakova<sup>1,2</sup>, S.N. Kulkov<sup>1,2</sup>

Tomsk State University, <sup>2</sup>Institute of Strength Physics and Material Science SB RAS, Tomsk. Russia

# P.S.B.33. DETERMINATION AND APPLICATION OF MATERIALS FOR AUTOMOTIVE TURBOCHARGERS

J. Lozanović Šajić<sup>1</sup>, V. Lozanović<sup>2</sup>

<sup>1</sup>Faculty of Mechanical Engineering, Innovation Center, Belgrade, Serbia <sup>2</sup>Coala – turbocharger service, Belgrade, Serbia

# P.S.B.34. THE CORELATION BETWEEN THE CHANGE IN THE DENSITY OF FREE ELECTRONS AND THE RELATIVE MAGNETIC PERMEABILITY OF THE AMORPHOUS ALLOY FE<sub>37.5</sub>NI<sub>17.5</sub>CR<sub>5</sub>CO<sub>15</sub>SI<sub>10</sub> UNDER THE INFLUENCE OF HEAT ACTION

<u>E. Gašanin</u>, D. Brajović, M. Dobričić, Z. Ristanović *Technical Colledge Čačak, Serbia* 

## P.S.B.35. CHARACTERIZATION OF IRON-COBALT BASED ALLOYS PROCESSED BY PIM ROUTE

<u>N. Mitrović</u><sup>1</sup>, B. Zlatkov<sup>2</sup>, H. Danninger<sup>3</sup>, B. Nedeljković<sup>1</sup>, A. Kalezić-Glisović<sup>1</sup>, A. Maričić<sup>1</sup>, S. Djukić<sup>1</sup>

<sup>1</sup>Joint Laboratory for Advanced Materials of SASA, Section for Amorphous, Systems, Technical Faculty Čačak, Čačak, University of Kragujevac, Serbia, <sup>2</sup>FOTEC Forsch & Technologietransfer GmbH, Wiener Neustadt, Austria, <sup>3</sup>Institute of Chemical Technologies and Analytics, Wien, Austria

# P.S.B.36. PLASTIC DEFORMATION MODELING OF SINGLE CRYSTALS WITH THE NaCI-TYPE LATTICE

D.V. Matsokin, I.N. Pakhomova, V.P. Matsokin V.N. Karazin Kharkov National University, Kharkov, Ukraine

#### P.S.B.37. STRUCTURE AND PROPERTIES OF ZIRCONIUM TUNGSTATE

E.S. Dedova<sup>1</sup>, S.N. Kulkov<sup>1,2</sup>

<sup>1</sup>Institute of Strength Physics and Material Science SB RAS, Tomsk, Russia, <sup>2</sup>Tomsk State University, Tomsk, Russia

#### P.S.B.38. PHONON THERMAL CONDUCTIVITY OF GRAPHENE

S.K. Jaćimovski <sup>1</sup>, <u>D.I. Raković <sup>2</sup></u>, J.P. Šetrajčić <sup>3</sup>,\*, S. Armaković <sup>3</sup>, V.M. Zorić <sup>3</sup>, B. Markoski <sup>4</sup>

<sup>1</sup>Academy of Criminalistic and Police Studies, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Electrical Engineering, Serbia, <sup>3</sup>University of Novi Sad, Faculty of Sciences, Department of Physics, Vojvodina – Serbia, <sup>4</sup>University of Novi Sad, Technical Faculty – Zrenjanin, Vojvodina – Serbia, \*Academy of Sciences and Arts of the Republic of Srpska – B&H

P.S.B.39. **OPTICAL SPECIFICITY OF TWOLAYERED MOLECULAR NANOFILMS**<u>J.P. Šetrajčić</u><sup>1,\*</sup>, D.Lj. Mirjanić<sup>2,\*</sup>, I.J. Šetrajčić<sup>1</sup>, D. Rodić<sup>1</sup>, S.S. Pelemiš<sup>3</sup>, B. Škipina<sup>4</sup>

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# P.S.B.40. SYNTHESIS OF FERRITE CORE/SILICA SHELL NANOPARTICLES B. Mojić<sup>1</sup>, K.P. Giannakopoulos<sup>2</sup>, V.V. Srdić<sup>1</sup>

Department of Materials Engineering, Faculty of Technology, University of Novi Sad, Novi Sad, Serbia, <sup>2</sup>Institute of Material Sciences, NCSR "Demokritos", Athens, Greece. Currently at the Institute of Microelectronics, NCSR "Demokritos", Athens, Greece

# P.S.B.41. THE INFLUENCE OF THE MICROSTRUCTURE ON THE DOMAIN STRUCTURE AND MAGNETIC PROPERTIES OF Nd-Fe-Al ALLOYS

<u>D. Derewnicka<sup>1</sup></u>, S. Arabasz<sup>2</sup>, E. Sieczkowska<sup>3</sup>, H. Krztoń<sup>2</sup>, B. Michalski<sup>4</sup>, W. Kaszuwara<sup>4</sup>, A. Wawro<sup>3</sup>

<sup>1</sup>Institute of Precision Mechanics, Warsaw, Poland, <sup>2</sup>Institute for Ferrous Metallurgy, Gliwice, Poland, <sup>3</sup>Institute of Physic Polish Academy of Science, Warsaw, Poland, <sup>4</sup>Warsaw University of Technology, Faculty of Materials Science and Engineering, Warsaw, Poland

# P.S.B.42. POROUS ALUMINA SINTERED FROM DIFFERENT GRAIN SIZE POWDERS

M.V. Grigoriev, S.N. Kulkov

Institute of Strength Physics and Materials Science of the Siberian Branch of RAS, Russia, Tomsk

# P.S.B.43. COROSION STUDIES OF NiMnGa SHAPE MEMORY ALLOYS IN VARIOUS COROSIVE ENVIRONMENTS

E. Szmidt<sup>1</sup>, M. Grobelny<sup>1</sup>, K. Sielicki<sup>2</sup>, R. Wroblewski<sup>2</sup>. M. Leonowicz<sup>2</sup>

<sup>1</sup>ITS, Warszawa, Polska, <sup>2</sup>Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland

#### P.S.B.44. MECHANOCHEMICAL SYNTHESIS OF Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub>

<u>D. Kosanović</u><sup>1</sup>, S. Filipović<sup>1</sup>, N. Obradović<sup>1</sup>, M. Mitrić<sup>2</sup>, S. Marković<sup>1</sup>, A. Maričić<sup>3</sup>, V. Pavlović<sup>1</sup>, M. M. Ristić<sup>4</sup>

<sup>1</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>The Vinča Institute, Condensed Matter Physics Laboratory, Belgrade, Serbia, <sup>3</sup>Technical Faculty Čačak, Čačak, Serbia, <sup>4</sup>Serbian Academy of Sciences and Arts, Belgrade, Serbia

#### P.S.B.45. ANTIOXIDATIVE CAPACITY OF COMMERCIAL BEERS FROM SERBIA

<u>D. Paunović</u><sup>1</sup>, S.S. Mitić<sup>1</sup>, A.N. Pavlović<sup>1</sup>, S.B. Tošić<sup>1</sup>, M.N. Mitić<sup>1</sup>, M.B. Stojković<sup>1</sup>, R.J. Micić<sup>2</sup>

<sup>1</sup>University of Niš, Faculty of Sciences and Mathematics, Department of Chemistry, Niš, Serbia, <sup>2</sup>University of Priština, Faculty of Sciences and Mathematics, Kosovska Mitrovica

# P.S.B.46. CHARACTERIZATION SOLID, VISCOELASTIC AND LIQUID MATERIALS BY OPTO-MAGNETIC SPECTROSCOPY

<u>B. Jeftić</u>, I. Hut, D. Mladenović, J. Munćan, Z. Golubović, D. Šarac, A. Tomić NanoLab, Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Serbia

## P.S.B.47. RIETVELD REFINEMENT OF BARIUM TITANATE STANNATE CRYSTAL STRUCTURE

<u>Lj. Veselinović<sup>1</sup></u>, M. Mitrić<sup>2</sup>, M. Vukomanović<sup>1</sup>, S. Marković<sup>1</sup>, D. Uskoković<sup>1</sup> <sup>1</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>2</sup>The Vinča Institute of Nuclear Sciences, Belgrade, Serbia

# P.S.B.48. DETERMINATION OF THERMAL CONDUCTIVITY OF THE INSULATION MATERIALS USING NUMERICAL CALCULATION OF THE PRESSURE INCREASE

M. Prvulović, <u>M. Ristić</u>, M. Prokolab, M. Kočić, A. Alil, Z. Milutinović, S. Budimir *Institute Goša, Belgrade, Serbia* 

# P.S.B.49. CHARACTERIZATION OF DIVERSE BIO-COMPOSITE MATERIALS BY INDENTATION, SIMULATION AND INVERSE ANALYSIS

V. Buljak, I. Balać, M. Milovančević

Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia

# P.S.B.50. KINETICS MODEL OF OXIDATIVE PROCESS IN BASIL-BASED SPREADS BY COLOUR ANALYSIS

L. Pezo, M. Pavlović, S. Ostojić, M. Kićanović, S. Zlatanović, O. Kovačević Institute of General and Physical Chemistry, Beograd, Serbia

# P.S.B.51. THE INCREASE OF REACTIVITY OF THE COPPER-NICKEL SULFIDE ALLOY BY TEMPERING

L. Udoeva, R. Gulyaeva, E. Selivanov, A. Vershinin,
Institute of Metallurgy, Ural Branch of Russian Academy of Sciences, Yekaterinburg,
Russia

#### POSTER SESSION III

Thursday, September 8, 2011, 20<sup>30</sup>-22<sup>00</sup>

#### SYMPOSIUM C: NANOSTRUCTURED MATERIALS

# P.S.C.1. LOW-TEMPERATURE ELECTRON TRANSPORT PROPERTIES OF CARBON NANOTUBES

V. Egorushkin, <u>N. Melnikova</u>, A. Ponomarev, N. Bobenko Institute of Strength Physics and Materials Science Siberian Branch of Russian Academy of Sciences, Tomsk, Russia

## P.S.C.2. MAGNETIC CRYSTALLITES ENCLOSED IN CARBON MATRIX FOR PROSPECTIVE BIOMEDICAL APPLICATION

M. Izydorzak, M. Leonowicz

Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland

# P.S.C.3. MULTIPLE SPIN DYNAMICS IN Co<sub>1+y</sub>Al<sub>2-y</sub>O<sub>4</sub> SPINEL DILUTED IN AMORPHOUS SiO<sub>2</sub>

<u>D. Milivojević</u><sup>1</sup>, B. Babić-Stojić<sup>1</sup>, V. Jokanović<sup>1</sup>, Z. Jagličić<sup>2</sup>, D. Branković<sup>1</sup>, N. Jović<sup>1</sup>, S. Čupić<sup>1</sup>, D. Kojić<sup>3</sup>

<sup>1</sup>Vinča Institute of Nuclear Sciences, Belgrade, University of Belgrade, Serbia, <sup>2</sup>Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenija, <sup>3</sup>Faculty of Mechanical Engineering, Belgrade, University of Belgrade, Serbia

# P.S.C.4. ACCELERATED POLYMORPHOUS TRANSFORMATION OF ALUMINA IMPED COPPER ALUMINATE SPINEL FORMATION

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# P.S.C.5. TRANSFOMATIONS AND MICROMECHANICAL INSTABILITY BEHAVIOR OF POROUS CERAMIC

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# P.S.C.6. THE ANALYSIS OF STABILITY OF THE ELECTROSPINNING PROCESS OF FORMING PVB-SiO<sub>2</sub> NANOCOMPOSITE FIBERS

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# P.S.C.7. PREPARATION, CHARACTERIZATION AND UP-CONVERSION OF Er<sup>3+</sup> DOPED YTTRIUM-LUTETIUM OXIDE NANOPHOSPHOR

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# P.S.C.8. MONODISPERSE LUMINESCENT PARTICLES OF $Y_{2-x}Gd_XO_3$ : Eu SOLID SOLUTIONS

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# P.S.C.9. SYNTHESIS AND CHARACTERIZATION OF NANOSTRUCTURED BOEHMITE POWDERS FOR OBTAINING TRANSITION GAMMA ALUMINA

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# P.S.C.10. NANOCRYSTALLIZATION OF GLASS IN THE SYSTEM Li<sub>2</sub>O·GeO<sub>2</sub>·P<sub>2</sub>O<sub>5</sub> S.D. Matijašević<sup>1</sup>, M.B. Tošić<sup>1</sup>, S.R. Grujić<sup>2</sup>, V.D. Živanović<sup>1</sup>, J.N. Stojanović<sup>1</sup>, J.D. Nikolić<sup>1</sup>, M.S. Djošić<sup>1</sup>

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# P.S.C.11. OPTICAL PROPERTIES OF NANOCOMPOSITE FILMS BASED ON Ag/PMMA SYSTEM

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# P.S.C.12. RHEOLOGICAL CHARACTERIZATION OF MAGNETORHEOLOGICAL FLUIDS WITH BIMODAL IRON PARTICLES

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# P.S.C.13. SHEAR THICKENING FLUIDS BASED ON NANOSIZED SILICA SUSPENSIONS FOR ADVANCED BODY ARMOUR

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# P.S.C.14. CHARACTERIZATION OF NANOSTRUCTURED POLYURETHANE ELASTOMERS VIA ATOMIC FORCE MICROSCOPY

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## P.S.C.15. MODIFIED THERMOPLASTIC IMPREGNATED MULTIAXIAL ARAMID FABRICS WITH NANOSILICA REINFORCEMENT

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# P.S.C.16. MECHANOCHEMICAL SYNTHESIS AND CHARACTERISATION OF NANOCRYSTALLINE BISMUTH SELENIDES (BiSe, Bi<sub>2</sub>Se<sub>3</sub>)

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# P.S.C.17. MECHANICAL SYNTHESYS OF MAGNESIUM BASED NANOCOMPOSITES

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# P.S.C.18. LOW TEMPERATURE MECHANICAL CHARACTERISTICS OF TI GRADE 2, PRODUCED BY DIFFERENT METHODS OF SEVERE PLASTIC DEFORMATION

E. Tabachnikova

B. Verkin Institute for Low Temperature Physics & Engineering, NASU, Kharkov, Ukraine

# P.S.C.19. ON THE KINETICS OF REACTIONS TAKE PLACE DURING MECHANOCHEMICAL SYNTHESIS OF W-Cu AND Mo-Cu NANOCOMPOSITES FROM THE OXIDE COMPOUNDS

A. Dolatmoradi, A. Rahmani, <u>Sh. Raygan</u>, H. Abdizadeh School of Metallurgy and Materials Engineering, College of Engineering, University of Tehran, Tehran, Iran

#### SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

## P.S.D.1. REMOVAL OF PHARMACEUTICALLY ACTIVE COMPOUNDS BY MESOPOROUS ZSM-5 ZEOLITE

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# P.S.D.2. THE ECO-FRIENDLY METHOD OF THE BIOACTIV COMPOUND EXTRACTION

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## P.S.D.3. NOVEL MECHANOCHEMICAL METHOD OF BIOPLASTICS MANUFACTORING FROM AGRICULTURE WASTES

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# P.S.D.4. IRRADIATION AGING OF CHLOROSULPHONATED POLYETHYLENE RUBBER BLENDS

G. Marković<sup>1</sup>, M. Marinović-Cincović<sup>2</sup>, V. Jovanović<sup>3</sup>, S. Samaržija-Jovanović<sup>3</sup>, J. Budinski-Simendić<sup>4</sup>

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## P.S.D.5. DIGITAL RADIOGRAPHY ON MONITORING OF CONCRETE PUMP MADE BY CARBOTECH COMPOSITE MATERIAL

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# P.S.D.6. ELECTRICAL PROPERTIES INVESTIGATION IN POLYSTYRÈNE/POLYANILINE COMPOSITES

D. Mezdour<sup>1</sup>, M. Tabellout<sup>2</sup>, S. Sahli<sup>3</sup>

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Mentouri, Constantine, Algérie

#### P.S.D.7. HUMATE MATERIALS FOR SOIL REMEDIATION

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# P.S.D.8. SEROTONIN CONTAINING POWDER MATERIALS FROM PLANT RAW O.I. Lomovsky<sup>1</sup>, M.P. Moshkin<sup>2</sup>

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# P.S.D.9. HEAVY METAL CONTENT DETERMINATION IN DOMESTIC PEACHES B.T. Stojanović, S.S. Mitić, M.B. Stojković, M.N. Mitić, J.Lj. Pavlović, I.D. Rašić Mišić

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#### P.S.D.10. THERMOOXIDATIVE STABILITY OF NANOSILICA-BASED UREA-FORMALDEHYDE HYBRID COMPOSITE WITH 4-CHLORO-3-NITRO-2H-CHROMEN-2-ONE

S. Samaržija-Jovanović<sup>1</sup>, V. Jovanović<sup>1</sup>, B. Dekić<sup>1</sup>, V. Dekić<sup>1</sup>, S. Konstaninović<sup>2</sup>, G. Marković<sup>3</sup>, M. Marinović-Cincović<sup>4</sup>

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#### **SYMPOSIUM E: BIOMATERIALS**

# P.S.E.1. SYNTHESIS, CHARACTERISATION AND BIOLOGICAL ACTIVITY OF A BIOLOGICALLY ACTIVE BRIDGED DIPHOSPHONIUM COMPOUND

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# P.S.E.2. IN VITRO ANTITUMORAL ACTIVITY OF PLATINUM(IV) COMPLEX WITH O,O'-DIPROPYL-(S,S)-ETHYLENEDIAMINE-N,N'-DI-2-(4-METHYL)PENTANOATE LIGAND

J.M. Vujić<sup>1</sup>, G.N. Kaludjerović<sup>2,3</sup>, B.B. Zmejkovski<sup>2</sup>, M. Milovanović<sup>4</sup>, V. Volarević<sup>4</sup>, N. Arsenijević<sup>4</sup>, S.R. Trifunović<sup>5</sup>

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# P.S.E.3. THE SWELLING BEHAVIOR OF THE POLY(METHACRYLIC ACID) HYDROGELS MODIFIED WITH DIFFERENT TYPE OF PECTIN

T.S. Radoman, E.S. Dzunuzović, S.J. Veličković Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

#### P.S.E.4. NANOINDENTATION HARDNESS OF ENAMEL

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## P.S.E.5 PARAMAGNETIC NANOPARTICLES IN THE REGENERATION OF THE REDUCED ALVEOLAR BONE DENSITY

Z. Ajduković<sup>1</sup>, <u>M.B. Petrović</u><sup>1</sup>, J. Milićević<sup>1</sup>, N. Djordjević<sup>2</sup>, N. Ignjatović<sup>3</sup>, V. Savić<sup>4</sup>, S. Najman<sup>4</sup>, D. Mihailović<sup>5</sup>, P. Vasiljević<sup>6</sup>, D. Uskoković<sup>3</sup>

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# P.S.E.6. THE INFLUENCE OF INITIATOR TYPE ON THERMAL PROPERTIES OF SYNTHESISED POLY(L-LACTIDE)

<u>I.S. Ristić</u><sup>1</sup>, J. Budinski-Simendić<sup>1</sup>, V. Jašo<sup>1</sup>, N. Vukić<sup>1</sup>, Lj. Nikolić<sup>2</sup>, S. Cakić<sup>2</sup>, O. Ilić<sup>2</sup>

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# P.S.E.7. AGGREGATION OF FULLERENOL NANO PARTICLES IN CELL MEDIUM RPMI 1640 WITH FETAL BOVINE SERUM

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## P.S.E.8. BIOLOGICAL ACTIVITIES AND PHYTOCHEMICAL SCREENING OF THE PLANT KITAIBELIA VITIFOLIA

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# P.S.E.9. BIODEGRADABLE CITRIC-ACID BASED POLYESTER ELASTOMERS FOR TISSUE ENGINEERING APPLICATIONS

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# P.S.E.10. HYDROTHERMAL SYNTHESIS OF ZnO NANOSTRUCTURES WITH DIFFERENT MORPHOLOGIES AND THEIR ANTIMICROBIAL ACTIVITY AGAINST Escherihia coli AND Staphylococus aureus BACTERIAL CUI TUDES

<u>A. Stanković</u><sup>1</sup>, Lj. Veselinović<sup>1</sup>, S. Marković<sup>1</sup>, S. Dimitrijević<sup>2</sup>, S. Skapin<sup>3</sup>, D. Uskoković<sup>1</sup>

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## P.S.E.11. CHITOSAN-POLYETHYLENE OXIDE FILMS FOR CONTROLLED DRUG RELEASE

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# P.S.E.12. THE FABRICATION OF ELECTROSPUN CHITOSAN NANOFIBER'S MAT WITH EMBEDDED SINGLE- AND MULTI-WALLED CARBON NANOTUBES

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## P.S.E.13. MONOMER ELUTION FROM EXSPERIMENTAL COMPOSITES WITH HYDROXYAPATITE FILLERS

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# P.S.E.14. STRESS-STRAIN RELATIONS BETWEEN POLYMER GEL MICROENVIRNMENT AND GOWING CELL CLUSTERS

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# P.S.E.15. CHARACTERIZATION OF FULLERENES THIN FILM ON GLASSES AND CONTACT LANCES BY UV/VIS /IR AND OPTO-MAGNETIC SPECTROSCOPY

<u>J. Šakota<sup>1</sup></u>, D. Stamenković<sup>2</sup>, N. Jagodić<sup>2</sup>, J. Munćan<sup>1</sup>, B. Jeftić<sup>1</sup>, L. Matija<sup>1</sup>, Dj. Koruga<sup>1</sup>

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# P.S.E.16. AFM/MFM INVESTIGATION OF FULLERENES THIN FILM ON GLASSES AND FULLERENE DOPED CONTACT LANCES

<u>I. Djuričić<sup>1</sup></u>, I. Mileusnić<sup>1</sup>, M. Tomić<sup>1</sup>, D. Stamenković<sup>2</sup>, N. Jagodic<sup>2</sup>, Lj. Petrov<sup>1</sup>, Dj. Koruga<sup>1</sup>

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# P.S.E.17. pH SENSITIVE COPPER/POLY(2-HYDROXYETHYL ACRYLATE/ITACONIC ACID) HYBRID HYDROGELS

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# P.S.E.18. THE EFFECT OF REACTION CONDITIONS ON BASIC STRUCTURAL PARAMETERS AND ELECTRICAL CONDUCTIVITY OF POLY(ACRYLIC ACID)-GELATIN COMPOSITE HYDROGELS

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## P.S.E.19. ELECTRODE-SKIN INTERFACE MODIFICATION: HYDRATION AND IONIC STRENGTH EFFECT

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# P.S.E.20. INFLUENCE OF PRODUCTION TECHNIQUES ON ELECTROCHEMICAL PROPERTIES OF THE Mg-3Al-1Zn ALLOY IN BODY-FLUID SOLUTION

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# P.S.E.21. THE ROLE OF PERIFERAL BLOOD CELLS IN THE INDUCTION OF ECTOPIC OSTEOGENESIS

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# P.S.E.22. SOLID STATE PROPERTIES AND ANTICANCER EFFECTS OF ARSENIC SULPHIDE NANOSUSPENSIONS

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# P.S.E.23. SYNTHESIS OF CORE-SHELL PARTICLES WITH BOTH FERITE AND SILICA SHELL AS SUPPORTS FOR ENZYME IMMOBILIZATION

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# Oral Presentation

PL.S.I.1.

## NANOSTRUCTURE PROCESSING OF ADVANCED BIOMATERIALS AND BIOSYSTEMS

J.Y. Ying

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Nanostructured materials are of interest for a variety of applications. Through controlled synthesis in reverse microemulsions, my laboratory has achieved polymeric nanoparticles for the glucose-sensitive delivery of insulin. These stimuli-responsive materials allow for the appropriate insulin delivery to diabetic patients only when their blood sugar levels are high, without the need for external blood sugar monitoring. We have also developed apatite-polymer nanocomposite particles for the sustained, zero-order delivery of protein therapeutics. By adsorbing valuable bone morphogenetic proteins on carbonated apatite nanocrystals that are then encapsulated within biodegradable polymeric microparticles, we are able to achieve controlled release of this growth factor for the bone healing process over an extended period of time.

In addition, nanostructure processing has been employed in artificial implant and tissue engineering applications. For example, nanocomposite processing has been applied to obtain orthopedic implants and bone scaffolds with superior mechanical strength and bioactivity. By combining microfabrication and nanotechnology, we have also created various microstructures in kidney-specific dimensions and shapes. These structures can be used as bioartificial renal assist microdevices, and may serve as three-dimensional templates for tissue engineering.

PL.S.I.2.

# USING THE TEAM MICROSCOPE TO INVESTIGATE THE ATOMIC STRUCTURE OF PARTICLES, DEFECTS AND INTERFACES IN MATERIALS

#### U. Dahmen

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Recent advances in aberration-corrected microscopy have made it possible to observe the structure and dynamics of materials with a new level of spatial and temporal resolution. By taking advantage of this capability, we have investigated the relationship between local atomic structure and behavior of interfaces and their defects. After a brief review of the TEAM project, this talk will highlight some recent applications of the TEAM microscope to the study of nanoscale particles, interfaces and topological defects in crystals. Examples will include short research summaries from a broad range of user projects involving graphene and energy-related materials. The major focus of this presentation will be the structure, glide and migration of highangle grain boundaries in gold, and the role of wetting in the formation of monodisperse coreshell particles by solid state reactions. Both of these issues rely critically on the ability to obtain atomic resolution images with a high ratio of signal to noise. Using aberration-corrected TEM and STEM imaging, we have observed the atomic structure and defects of several special grain boundaries in Au. Direct observations of such defects show that they involve highly correlated motion of groups of atoms and suggest that these are related to the mechanism of boundary migration. This talk will summarize recent advances in our understanding of these grain boundaries using time-resolved STEM and TEM imaging techniques and quantitative comparison to atomistic models. Finally, this presentation will outline opportunities for future research and instrument development based on aberration-corrected electron microscopy.

PL.S.I.3.

## CHARACTERIZATION AND APPLICATION OF GRAPHENE AND NANOSTRUCTURED BORON NITRIDE

#### A. Zettl

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We have explored different synthesis routes for graphene, BN nanotubes (BNNTs), and few-atomic-layer BN sheets (BNS), including hybrid structures that contain carbon and BN. Characterization of these materials is via high resolution TEM and via transport measurements, including magnetotransport to 18T. Grain boundaries are mapped using electron diffraction in STEM mode and also dark-field imaging in conventional TEM. Atomic resolution imaging using the TEAM microscopes at Berkeley has also been performed. The defect structure, including atom dynamics, are markedly different in BN and carbon-based nanostructures. We explore the mechanical robustness of graphene and BN sheets, including easy and hard directions for ripping. Graphene is folded to form "grafold", and layers of graphene and/or BN are sandwiched to form "veils" and "sandwiches", which can immobilize foreign atomic, molecular, or nanocrystalline species.

PL.S.I.4.

#### BIOMIMETICS: LESSONS FROM NATURE

Bh. Bhushan

Ohio Eminent Scholar and The Howard D. Winbigler Professor,
Director, Nanoprobe Laboratory for Bio- & Nanotechnology and Biomimetics,
The Ohio State University, Columbus, Ohio, USA

Nature has developed materials, objects, and processes which function from the macroscale to the nanoscale. These have gone through evolution over 3.8 billion years. The emerging field of biomimetics allows one to mimic biology or nature to develop nanomaterials, nanodevices, and processes<sup>1,2</sup>. Properties of biological materials and surfaces result from a complex interplay between surface morphology and physical and chemical properties. Hierarchical structures with dimensions of features ranging from macroscale to the nanoscale are extremely common in nature to provide properties of interest. Molecular scale devices, superhydrophobicity, selfcleaning, drag reduction in fluid flow, energy conversion and conservation, high adhesion, reversible adhesion, aerodynamic lift, materials and fibers with high mechanical strength, biological self-assembly, anti-reflection, structural coloration, thermal insulation, self-healing, and sensory aid mechanisms are some of the examples found in nature which are of commercial interest. This talk will provide a broad overview of four selected objects of interest found in nature and applications under development or available in the marketplace. These will include Lotus Effect used to develop superhydrophobic and self-cleaning surfaces with low adhesion<sup>3-5</sup>, Rose Petal Effect used to develop superhydrophobic surfaces with high adhesion<sup>6</sup>, Gecko Adhesion to develop surfaces with reversible adhesion, and Shark Skin to develop surfaces with low fluid drag<sup>8</sup>.

<sup>&</sup>lt;sup>1</sup>Bhushan, B., "Biomimetics: Lessons from Nature - An Overview," *Phil Trans. R. Soc. A* **367**, 1445-1486 (2009).

<sup>&</sup>lt;sup>2</sup>Bhushan, B., *Springer Handbook of Nanotechnology, 3<sup>rd</sup> edition*, Springer-Verlag, Heidelberg, 2010.

<sup>&</sup>lt;sup>3</sup>Nosonovsky, M. and Bhushan, B., *Multiscale Dissipative Mechanisms and Hierarchical Surfaces: Friction, Superhydrophobicity, and Biomimetics*, Springer, Heidelberg, Germany, 2008.

<sup>&</sup>lt;sup>4</sup>Bhushan, B. Jung, Y. C. and Koch, K., "Micro-, Nano-, and Hierarchical Structures for Superhydrophobicity, Self-Cleaning and Low Adhesion", *Phil. Trans. R. Soc. A* 367, 1631-1672 (2009).

<sup>&</sup>lt;sup>5</sup>Bhushan, B. and Jung, Y. C., "Natural and Biomimetic Artificial Surfaces for Superhydrophobicity, Self-Cleaning, Low Adhesion, and Drag Reduction," *Prog. Mater. Sci.* **56**, 1-108 (2011).

<sup>&</sup>lt;sup>6</sup>Bhushan, B. and Her, E.K., "Fabrication of Superhydrophobic Surfaces with High and Low Adhesion Inspired from Rose Petal," *Langmuir* **26**, 8207-8217 (2010).

<sup>&</sup>lt;sup>7</sup>Bhushan, B., "Adhesion of Multi-level Hierarchical Attachment Systems in Gecko Feet," (invited), *J. Adhesion Sci. Technol.* **21**, 1213-1258 (2007).

<sup>&</sup>lt;sup>8</sup>Dean, B. and Bhushan, B., "Shark Skin Surfaces for Fluid Drag Reduction in Turbulent Flow – A Review," *Phil. Trans. R. Soc. A* **368**, 4775-4806 (2010)

PL.S.I.5.

#### AN UP-DATE ON FACILITIES FOR NANOCHARACTERIZATION

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During the last five years or so, our institution has put significant thought and effort into providing multi-user facilities for its scientific and technical community. This paper will describe this development and the outcome in terms of user numbers, breadth of applications, financial considerations etc. At the same time our aim is to provide both routine characterization and the most advanced sophisticated tools. Strategies for optimizing this effort will be described, including some examples of recent results.

PL.S.I.6.

#### M<sub>2</sub>O<sub>3</sub>(ZnO)<sub>n</sub> NANOWIRES FOR THERMOELECTRIC APPLICATIONS

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Some complex superlattices in nanostructures contain periodic compositional and structural features, typically on the nanometer scale, making them promising materials for thermoelectric applications. Recently we discovered a novel method to produce  $M_2O_3(ZnO)_n$  polytypoid nanowires (M=In, Ga, Fe,...) by a facile solid state diffusion process [1], in agreement with the theoretical prediction that it is possible to increase the material-dependent figure of merit, zT, by using low dimensional materials [2], attributed to electronic band structure changes and enhanced interface phonon scattering. Using atomic resolution Z-contrast STEM imaging we performed a detailed structural analysis on the  $M_2O_3(ZnO)_n$  nanowires, unambiguously determined the location of indium within the structure and to evaluate lattice strain and the presence of defects. Based on this analysis we propose that the superlattice structure is generated through a defect-assisted process. One of the greatest advantages of this novel synthesis is the ability to tune the nanoscale features of the polytypoid wires by simply adjusting the amount of metal precursor. We also performed a quantitative analysis of the change in superlattice inclusion density and periodicity with metal deposition. This will enable future studies on structure-dependent thermoelectric properties and possibly lead to further enhancements in thermoelectric efficiency. [3]

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- [2] L.D. Hicks and M. S.Dresselhaus, *Phys. Rev. B*, 47 (1993) 16631.
- [3] This work was performed at the National Center for Electron Microscopy, LBNL, Berkeley, which is supported by the Director, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. VR acknowledges support by the Ministry of Education and Science of the Republic of Serbia, under project No. 172054 and Nanotechnology and Functional Materials Center, funded by the EC FP7 regpot project No. 245916.

O.S.A.1.

#### SONOELECTROCHEMISTRY – A VERSATILE TOOL FOR THE PREPARATION OF NANOMATERIALS

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Sonoelectrochemistry, the application of ultrasound in electrochemistry has become increasingly popular in the past decade, especially in the field of materials science because of its potential in the production of nanomaterials, metals, alloys and composites. The major effects of ultrasound in electrochemical reactions are the enhanced mass transport due to acoustic streaming, influence of cavitation on reaction mechanism and surface cleaning and erosion. Electrochemical experiments can be performed by positioning the horn face to face to the working electrode with a distance between 1-80 mm, or by using the ultrasonic horn generating the ultrasound itself as the cathode, which is especially suitable for the production of nanopowders. Both approaches are discussed along with the possibility to use an Electrochemical Quartz Crystal Microbalance to monitor the process.

O.S.A.2.

#### SYNTHESES AND CHARACTERIZATIONS OF LiFePO<sub>4</sub> POWDERS

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The olivine type compositions LiMPO<sub>4</sub> (M = Fe, Mn, Co) are among the most attractive materials for the positive electrode of lithium-ion battery. The benefits of using LiFePO<sub>4</sub> are excellent cycle life, high structural stability, low cost and environmental friendliness. Here will be presented our efforts to obtain LiFePO<sub>4</sub> powders through several synthesis methods. The differences in phase purity, microstructure, morphology, and electrochemical performances of synthesized powders were investigated by using several techniques such as X-ray powder diffraction, scanning electron microscopy, galvanostatic cycling, Mossbauer spectroscopy, and thermogravimetry. It was found that carbon coated, nanostructured particles with minimal structural imperfections showed the best electrochemical performances.

O.S.A.3.

#### LITHIUM IRON PHOSPHATE MESOCRYSTALS FOR LITHIUM-ION BATTERIES

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Mesocrystals are 3D ordered nanoparticle superstructures with new chemical and physical properties arising from their unique hierarchical mesostructure. These specific morphologies composed of nanoscaled hierarchically assembled units can be considered as possible future high rate capability electrodes for Li-ion batteries due to their internal framework which can provide high accessibility for the electrolyte. Since its discovery, olivine LiFePO<sub>4</sub> has been highlighted as one of the most promising cathode material for large size Li-ion batteries due to its high stability, high power and low cost. However, the main drawback of LiFePO<sub>4</sub> as electrode material lies in its low intrinsic and electronic conductivity. In this context, extensive research has been done to address present problem including reduction of the particle size, coating with conductive agents and most recently via the synthesis of porous LiFePO<sub>4</sub> monoliths. Here, we present a simple up-scalable solvothermal template-free low temperature route for the preparation of novel and exciting mesocrystals of LiFePO<sub>4</sub> coated in situ with Nitrogen-doped carbon. Nitrogen-doping in carbon materials is known to dramatically increase the conductivity due to its electron excess as a result of possible overlapping of the conduction and valence bonds. This synthesis method can also be extended to other phospho-olivines. X-ray diffraction followed by Le Bail full profile refinement using Fullprof® software of the asprepared powders showed the existence of a single crystalline phase of LiFePO

O.S.A.4.

#### SINTERING OF DEFECT-FREE FUNCTIONALLY GRADED BIOMATERIALS

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Functionally graded materials (FGMs) with a gradient of chemical, electrical, mechanical and/or biological properties are very attractive because of their superior features compared to conventional materials. It is known that implanted hydroxyapatite (HAp) scaffolds with a porosity gradient which mimicked the architecture of natural bone, induce rapid bone ingrowths into the high-porosity portion and withstand physiological mechanical stresses through the low-porosity region.<sup>1</sup>

Here, three, four and five component hydroxyapatite functionally graded materials (HAp-FGMs) were designed and examined. HAp powders with different stoichiometry denoted as SHAp (stoichiometric, Ca/P = 1.67) and CDHAp (calcium defficient, Ca/P = 1.62) were used. These two powders were chosen since they show different sinterability in the same sintering conditions, yielding different microstructure (density and average grain size) and also mechanical properties which is necessary for tailoring of appropriate functionally graded biomaterials. It is known that during sintering of FGMs composed of powders which show different shrinkage extents, as well as different final density, excessive shape distortion, warping, delamination, cracks and microstructural damages in the FGMs could be produced. Thus, to achieve high-quality graded biomaterials with appropriate functionality without above listed disadvantages, we applied moderate sintering conditions through two step sintering (TSS) process. Furthermore, TSS method was chosen since significantly improved microstructural characteristics of HAp and BCP could be obtained. So, layered samples, produced by powderstacking method and uniaxially-pressing process, were transformed in HAp-FGMs by TSS: the samples were heated up to 900 °C and after retention for 5 min the samples were cooled down to 850 °C and kept for 20 h. The microstructure and Ca/P ratio of the prepared HAp-FGMs were examined by FESEM and EDS methods; mechanical characteristics were analyzed by nanoindentation.

1. Tampieri A, Celotti G, Sprio S, Delcegliano A, Franzese S. Porosity-graded hydroxyapatite ceramics to replace natural bone. *Biomaterials* 2001, **22**, 1365–70.

O.S.A.5.

#### MECHANOCHEMICAL SULPHIDIZATION AND SULPHUR COATING OF NON-FERROUS METAL-OXIDES IN FLY-ASH AND THEIR RECOVERY BY FLOTATION

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Fly ash is one of the residues produced from waste combustion facilities, and its amount reaches 5-billion tons every year in our country. It contains non-ferrous metals oxides such as CuO, ZnO and PbO, which would be useful materials when they are recovered from the ash. The amount ratio of such metal oxides in fly ash is approximately 10 to 30wt%, depending on facilities, so that it would be of great interest to recover them from the fly ash. It is easy to recover such nonferrous sulphide by flotation, though such oxides are very difficult to recover by this separation technique. Thus, we have attempted to sulphidize the metal oxides mechanochemically, in order to recover them by flotation technique.

First of all, the nonferrous metal oxide (CuO, ZnO and PbO) was mixed with sulpher (S) under the presence of reducer (Fe powder) to grind in dry condition by a planetary ball mill at different conditions. The milled powders were characterized by different analytical methods such as XRD and XPS to make sure the sulphidisation in part of the oxide particles. We have discussed the results from the thermodynamic point of view. The milled product was subjected to flotation to float the oxide powder from the product. The reason why the recovery of the oxide particles by the flotation has increased is due to sulphidization and oxide particles coated with sulphur by the grinding. It has been found that the grinding causes sulphydization and sulphur coating of the metal oxide particles, and this phenomena are enhanced with an increase in grinding periods of time and rotational speed of the mill.

Keywords: Grinding, Sulphidization, Sulphur Coating, Flotation, Non-ferrous Metal Oxide, Fly-ash.

O.S.A.6.

# THE <sup>57</sup>FE-O COMPLEXES – MÖSSBAUER PROBES TO STUDY NANOSTRUCTURED MATERIALS

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The localization of Fe atoms in mechanically alloyed and followed by annealed Mo powder composite containing 8 at. % O at boundaries of the Mo grains has been investigated by Mössbauer spectroscopy on impurity <sup>57</sup>Fe isotope atoms (1 at. %), X-ray diffraction, Auger spectrometry, and ab initio calculation using the FP LAPW (WIEN 2k) method. The presence of oxygen in the boundaries of the bcc Mo grains leads to an extraordinary large isomer shift (2.0 mm/s with respect to  $\alpha$ -Fe) for the grain boundary component in the Mössbauer spectrum. With the Mo-O-Fe solid solution formation under mechanical alloying, the Fe atoms localized in substitutional positions yield two Mössbauer spectra with close isomer shifts of 0.04-0.06 mm/s but with the different line width, 0.45 and 0.69 mm/s. Besides, it has been found that the Mössbauer spectrum of Fe atoms in the cores of dislocations is characterized by the isomer shift of 0.60 mm/s. Influence of the number of O atoms in the environment of an Fe atom on its isomer shift has been confirmed by the ab initio calculations. As a result, the following three structural components have been identified in the mechanically activated system: a grain boundary and distorted close-to-boundary zones with common name "interface" and a grain with a perfect (defect-free) structure. For powder nanostructured (~ 10 nm) materials subjected to an intensive mechanical treatment in a planetary ball mill, widths of the unrelaxed grain boundary and interface have been experimentally estimated as 0.2 and 1 nm, respectively. This work has been supported by the Russian Fund for Basic Research (project No. 10-03-00077).

O.S.A.7.

#### NANOPOROUS ANODIC ALUMINA FILMS: INVESTIGATION OF GROWTH AND MORPHOLOGY EVOLUTION

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Nanoporous anodic alumina films can possess cylindrical pores with uniform size distribution and high pore density. Such films may be regarded as perfect matrixes for synthesis of one-dimensional nanostructures, microporous filters, separation membranes and preparation of functional composite materials. In present work we attempted to improve the regularity of the pores' arrangement, to control the pore size and the film thickness. Morphology evolution was studied by high-resolution electron microscopy, scanning electron microscopy and ellipsometry. Films with controlled morphology were obtained by fine tuning the anodization voltage, the current density, the temperature, the acid used, the pH of the electrolyte and the time of anodizing. A mechanism of pore growth is also discussed.

O.S.A.8.

#### EVAPORATION FROM LIQUID FILMS IN SOLID-LIQUID-GAS SYSTEMS

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Motivated by physical applications we consider a mathematical model describing the evaporation process in solid-liquid-gas systems with two moving boundaries of the phase transition. An alkali metal generator with a working substance in the form of the intermetallic compound and evaporation of a volatile component into vacuum is considered. Explicit analytical solutions of the problem under consideration are constructed in three different geometries of the process. We demonstrate that the evaporation boundary moves much slower than the dissolution boundary and the liquid layer thickness increases with time. The role of the evaporation coefficient on the evaporation stream and nonlinear dynamics of the process is studied.

O.S.A.9.

# SOLVENT-FREE MICROWAVE ASSISTED SYNTHESES OF AMINO ACID DERIVATIVES

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Microwave (MW) irradiation presents a powerful tool toward organic reactions. Solventfree microwave assisted synthesis has attracted a considerable amount of attention in recent years. Though the probability of an interaction between two solid reagents is restricted, such a reaction may occur when liquid phase of melting reagent (as one as both) appears under MW irradiation. We have investigated the microwave assisted syntheses of imide derivatives of amino acids. Imide derivatives are an important class of chemical substances due to their synthetic applications as well as physiological properties. Glycine and  $\gamma$ -aminobutyric acid (GABA) are known to act as neurotransmitters in the brain, and these amino acids including their phtalimides possess anticonvulsant properties as it was shown. We have studied the interaction of phthalic anhydride and glycine under solvent-free conditions as the model system. The reactions have been carried out in a Single-Mode Microwave reactor Discover S-Class equipped with temperature, pressure and power control system. The heating rate of each reactant — phthalic anhydride and glycine separately was studied under MW activation. The changing of the temperature rate in dependence on microwave irradiation power was monitored. It was found that a sharp increase in heating rate in 30-40 times occurs around the melting points of the products, presumably due to an increase in polarity associated with the change from the solid to the liquid phase. After many tests we have found the reaction conditions as the two steps way: at the first step the solid reagents were hold under the temperature, when phtalic anhydride melted, and after that the reaction mass was hold additionally under higher temperature, in accord with the melting point of amino acid reacted. Using such reaction conditions the series of phtalimide derivatives of amino acids has been obtained under microwave irradiation in solvent-free format.

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O.S.A.10.

# SYNTHESIS AND CHARACTERIZATION OF $Hf_{1-x}Y_xO_{2-\delta}$ SOLID SOLUTION NANOCRYSTALS

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Solid solution nanoparticles with composition  $Hf_{1-x}Y_xO_{2-\delta}$  (x = 0, 0.05, 0.1, 0.15 and 0.2) were produced via the metathesis treatment. The obtained powders were characterized by means of XRD, DTA, Elypsometry, SEM, BET and Raman scattering. It was demonstrated that the proposed synthetic technique led to the formation of a  $Hf_{1-x}Y_xO_{2-\delta}$  solid solution with thermodynamically metstable phases depending on incorporated  $Y^{+3}$  ion. Yttrium dopant serves effectively to induce a phase transformation from monoclinic to the cubic polymorph, even at temperature less than 600 °C.

O.S.A.11.

# "MECHANOCHEMICAL" NANO-Si. METHODS OF PREPARATION, DEFECT STRUCTURE AND REACTIVITY

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Mechanical destruction is one of method for preparation of fine powder of Si. Under standard method of mechanical activation of individual Si, the maximal specific surface area S is close to 25 m<sup>2</sup>/g and an average particle size is equal to 100 nm. The new mechanochemical method of nano sized Si (n-Si) preparation is developed. The idea of the new method is mechanochemical formation of nanocomposites Si/X (X=graphite, h-BN) followed by dissolving of second component X. Under the ball milling of mixture of brittle Si and flaky additives X the nanocomposites forms, in which particles of n-Si separated from each to other by molecules of X. The optimal concentration of additives X and the optimal dose of mechanical treatment for preparation of n-Si with minimal sizes are found. Using the new method it is possible to prepare nano particle of Si with 30 nm size (S=90 m<sup>2</sup>/g). The defect structure and reactivity of n-Si, prepared by new method (1) are compared with n-Si, prepared by standard method of mechanical activation of individual Si (2), by plasma method (3) and by thermal decomposition of silane (4). The particles size is determined by sorption (BET equation), SEM and TEM, coherent scattering regions (CSR) and dislocation concentration is estimated by XRD method, point defects are characterized by optic and electron paramagnetic resonance methods. The uniqueness of "mechanochemical" n-Si, (methods 1 and 2) in comparison to n-Si, prepared by other methods (3,4) is in higher concentration of dislocation and point defects. Thermal stability of main defects (outer surface, CSR, concentration of dislocations and point defects, etc.) is compared for different n-Si under annealing in inert environment and in oxygen. The reactivity of n-Si is controlled by the rate of thermal oxidation. The thermal oxidation is measured by TG and DSC methods with heating at constant velocity. The oxidation of n-Si takes place in wide temperature range from 300-400°C to 1200°C. There are three stages of n-Si oxidation: low, intermediate and high-temperature stages. The behavior of each stage oxidation depends on the methods preparation of n-Si and defect structure of samples. The work was carried out under financial support of RFBI (grants 10-03-00942a, 10-03-00909a, 09-03-00409a) and Program of Presidium RAS 7P.

O.S.A.12.

# SELECTIVE MICROWAVE HEATING OF COMPOUNDS, INTERCALATED INTO THE INTERLAYER SPACE OF POLIFLUORODICARBON

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Any systematic studies have not been carried in the field of microwave chemistry of intercalation compounds based on layered inorganic matrices up to now. However intercalation compounds are of great interest for the production of new nanocomposite functional materials and graphene. Thermal decomposition of volatile metal compounds intercalated into layered matrix leads to the formation of nanoparticles of metals or to metal oxides. Layered intercalate operates in this case as a two-dimensional nanoreactor.

We have carried out investigations on peculiarities of microwave heating of various chemical compounds. Studies were conducted with a microwave system Discover-S-Class, clocked at 2450 MHz with a controlled power microwave exposure from 0 to 300 Watts. The results of experiments on the heating of intercalated compounds with chlorine trifluoride and acetone, acetonitrile, benzene and carbon tetrachloride are obtained. It has been established that microwave energy deposition is determined by the complex dielectric permeability of the compounds (the presence of a dipole moment and its mobility) intercalated into the interlayer spaces of the matrix. It was shown that the decomposition of the matrix with the formation of nanostructured carbon occurs due to microwave energy absorption. The temperature for carbon formation under microwave irradiation is essentially lower in comparison with traditional convection heating.

We have investigated the characteristics of microwave heating of organic solutions of volatile metal compounds intercalated into the matrix of polifluorodicarbon. The features of the decomposition of intercalated compounds of fluorinated graphite with solutions of volatile compounds of metals with organic ligands at different levels of microwave exposure have been investigated. It was shown that the ability of a substance to absorb the energy of microwave radiation is determined either on the electronic or ionic conduction or displacement currents caused by the polarizability of the substance in the field of electromagnetic wave. In the absence of conduction currents in the materials used, the energy from the alternating electromagnetic field can be attributed to the ability of substances to the polarization.

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O.S.A.13.

# SIZE EFFECT FOR MODEL Ag/HOPG CATALYSTS IN THE REACTION OF ETHYLENE EPOXIDATION

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Series of the model Ag/HOPG catalysts with narrow silver particle size distribution (6, 40 and 200 nm) were prepared using evaporation-deposition procedure and studied in ethylene epoxidation reaction using combined *in situ* high pressure X-ray photoelectron spectroscopy (up to 0.5 mbar) and proton transfer mass spectrometry (PTR-MS). Simultaneous presence of two oxygen states on silver - nucleophilic (BE = 529 eV) and electrophilic (BE = 531 eV) - is the necessary condition for ethylene oxide to be detected (40 nm Ag particles). Sample with electrophylic oxygen (smaller Ag particles) was inactive, while for the sample with larger silver particles, the absence of the measurable signal of ethylene oxide in PTR-MS can be explained by low concentration of surface silver atoms.

O.S.B.1.

# THE RELAXATIONAL MODEL OF DOUBLE ELECTRIC LAYER IN DISTURBED CRYSTAL POTENTIAL RELIEF ON SUPERIONIC/ ELECTRONIC CONDUCTOR POLARIZED HETEROJUNCTIONS

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The phenomenological model that deals with a formation of double electric layer (DEL) in a disturbed (crystal) potential relief (DPR) on the electronic conductor (EC)/solid electrolyte (SE) polarized heterojunction is proposed. In the DPR- model, the behavior of DEL under strong external influences is connected with relaxation processes that strongly affect on the characteristics of all-solid-state nanoionic devices [1], e.g. supercapacitors. In the considered case, SE belongs to a class of advanced superionic conductors (AdSICs) [2]. The DPR-model postulates that on the structurally imperfect AdSIC/EC interface the depth  $(\eta)$  of potential wells for mobile ions can significantly exceed ones in the AdSIC bulk. The  $\eta$  difference induces the electrostatic "condensation" - the change of mobile ion distribution function, i.e. gradual transitions of mobile ions from non-equilibrium crystal positions to ones with lower electrostatic energy (large  $\eta$  values) at the EC interface region. The model is based on three assumptions discussed in [3-5]: (i) the formation of an atomically sharp AdSIC/EC interface, (ii) EC wave function penetration into AdSIC with the formation of charge distribution equivalent to an atomically thin DEL, and (iii) strong shift polarization effect (large values of permittivity k) of mobile ions of AdSIC. The model simulates the fast and slow relaxation and the response of DEL on weak and strong current densities ( $\delta_i$ ). The method of impedance spectroscopy (widely used for a study of electrochemical systems) describes and classifies electrochemical reactions in the terms of equivalent electric circuits (EECs). Within the framework of the DPR- model, we conclude that the criterion of small external influences on the polarized AdSIC/EC heterojunctions is usually used wrong in the impedance spectroscopy (for instance, [6]). The true general form of the criterion is: (i) capacitor (C-component) of EEC imposes restriction (from the bottom) on a generation (recombination) rate of charge carriers in the DEL; (ii) Ccomponent in EEC imposes restriction (from the top) on  $\delta_l$ ; (iii) EEC with C-component, for which there is not specified the top limit on  $\delta_l$  has no physical meaning. The frequency-capacity characteristics of nanoionic supercapacitors (experimental devices were created in IMT RAS) are analyzed in the terms of DPR-model. The prospects of nanoionic supercapacitor applications [2-5] are briefly considered in the report.

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O.S.B.2.

# THE INTERFACES IN SUPERIONIC CONDUCTORS AS NEW SENSITIVE MATERIAL FOR PERFORMANCE OPTIMIZATION OF NANOIONIC DEVICES

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Due to ongoing miniaturization in many hi-tech applications the interfaces become key elements determining the total properties of nanosystems (NSs) and the performance of micro-, nano-sized devices. In general, interfaces are non-equilibrium defects, but we can speak about local metastable equilibrium of a certain stationary interface under certain external conditions. Because the interface structure drastically differs from the bulk, therefore a central goal is the control of interfaces to atomic dimensions. By nature, NSs are open thermodynamic systems and their treatment is carried out under non-equilibrium conditions, therefore the evolution of a system during synthesis occurs in conditions far from equilibrium and the driving force of the process can be the system tendency to a minimum of entropy production near a stationary state]. From this point of view, the formation of low energy coherent (or semicoherent) interfaces in NSs seems predetermined. Obviously, the synergy processes of structural self-organization which lead to formation of a certain type of low-energy interfaces responsible for "unique" properties of a final material will have a pivotal value in NSs [1,3]. In the report the crystal interface engineering methods and thermodynamic considerations are applied to NSs of advanced superionic conductors (AdSICs) [2,4,5]. The crystal structure of AdSICs is close to optimal for fast ion transport (FIT), however it is disturbed on arbitrary heteroboundaries, therefore, FIT conservation in NS of AdSICs requires stable and structurally perfect interfaces. Stabilizing the right bandgap is necessary to induce superionicity. Fundamental challenge is conservation of FIT at functional AdSIC/electronic conductor (EC) heterojunctions. In the report an attempt has been made to integrate the model of double electric layer (DEL) on SE /EC polarized interface with structural model of low energy coincidence (coherent or semicoherent) that is simultaneously minimize both electrostatic and strain energy of interface region in the complementary manner. The basic crystallochemical concepts (electronegativity, the softness/hardness of bonding, connected with polarizability and energy gap, etc.) and algorithms of searching for low energy, symmetry preferable interfaces in NSs on the AdSIC basis [2] are presented. Some atomic models of stable and structurally perfect AdSIC/EC interfaces are simulated. The influence of the AdSIC/EC interface on the performance optimization of nanoionic supercapacitors [5] is discussed.

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O.S.B.3.

# DEVELOPMENT OF BORON HYDRIDES MATERIALS FOR HYDROGEN STORAGE

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Boron hydrides are candidate for hydrogen storage material because of its high gravimetric hydrogen density. Ammonia borane (NH<sub>3</sub>BH<sub>3</sub>) is one of the most attractive hydrides owing ti its hydrogen density (19.5 wt%). Sodium borohydride (NaBH<sub>4</sub>) attracts attention since the late 1999s because it is a quite stable compound storing 10.8 wt% of hydrogen. Stored hydrogen can be can be released by thermolysis or catalyzed hydrolysis, both routes having advantages and issues. Today, most of the published papers about the NaBH<sub>4</sub> hydrolysis deal with improvement of catalytic materials In this work we have studied the formation of cobalt boride depending on the nature of the reducing agent (NaBH<sub>4</sub>, NH<sub>3</sub>BH<sub>3</sub>), and the initial cobalt compound (CoCl<sub>2</sub>, Co<sub>3</sub>O<sub>4</sub>), as well as their activity in the hydrolysis of NaBH<sub>4</sub> and NH<sub>3</sub>BH<sub>3</sub>. Samples have been characterized by magnetic susceptibility method, FTIR, XRD, TEM. Through a thermal decompomposition of ammonia borane, 2.2 equiv. of hydrogen can be released from NH<sub>3</sub>BH<sub>3</sub> up to 473 K. In this work it was showed that loading NH<sub>3</sub>BH<sub>3</sub> into mesoporous carbon or titanium oxide can benefit its thermal decomposition of which the temperature threshold for hydrogen release and the volatile by-products are absent or notably lower than those for neat NH<sub>3</sub>BH<sub>3</sub>

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O.S.B.4.

# THE STUDY OF THE INTERFACIAL COATINGS ON REINFORCED CARBON AND SIC FIBERS FOR HIGH-TEMPERATURE COMPOSITES

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There is a great interest in the research and development of ceramic matrix composites (CMC's) reinforced by carbon or SiC fibers for a variety of high-temperature, high-stresses applications in aerospace, hot engine and energy conversion systems. For CMC's the property of fiber/matrix interface is one of key factors that determine the materials performance. A "weak" interphase layer 200-300 nm in size is required between the reinforcing fiber and the matrix for tough mechanical behavior. The most common interphases, pyrocarbon and boron nitride themselves and in combination with SiC oxidize at relatively low temperatures. Considerable effort has been exerted to improve the interphase oxidation resistance. Among alternative interphases the refractory oxide-based systems are considered as the most promising ones. The purpose of this work is to develop and to characterize the interfacial coatings for new generation SiC and carbon fibers for CMC's. As interfacial coatings, the refractory carbides and oxides, including stabilized zirconia, have been investigated. The surface chemistry, morphology, composition, topography, roughness, local mechanical and adhesive properties of interphases were evaluated by different analytical techniques, including high resolution scanning electron microscopy combined with energy-dispersive spectroscopy, X-ray photoelectron spectroscopy, X-ray analysis, atomic-force microscopy, Raman spectroscopy. Direct adhesion force mapping measurements on as-received and coated fibers were performed by atomic force microscopy. Mechanical properties of the fiber/matrix interface in composites were investigated using an indentation method. The obtained results provide new insights into composite mechanical performance.

O.S.B.5.

# ALUMINOSILICATE INORGANIC POLYMERS: THE EFFECTS OF POLYPROPYLENE FILLERS ON MECHANICAL BEHAVIOR

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Aluminosilicate inorganic polymers (AIP), are promising building material due to their high compressive strength. However, low flexural strength limits their applications. This work is aimed on tailoring flexural strength by incorporation of short polypropylene (PP) fibers at volume fraction from 1 to 25 %. It has been shown, that the flexural strength increases with increasing volume fraction of the fibers. On the other hand, addition of lower amount (< 10 %) of the fibers leads to a decrease in compressive strength. With further increasing the fiber loading, the compressive strength increases, reaching the value of the non-reinforced sample at the highest fibre loading. Simultaneously, the effects of PP particles on the ultimate mechanical behavior were studied.

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O.S.B.6.

# STRUCTURAL TRANSFORMATION IN La<sub>1-x</sub>Ca<sub>x</sub>MeO<sub>3</sub> (Me=Mn, Fe) PEROVSKITES DURING METHANE OXIDATION PROCESS

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High temperature X-ray in the air/vacuum, HRTEM, TA,  $H_2$ -TPR and BET for as prepared (via the Pechini route) and tested in methane oxidation (1% methane+9% $O_2$  + 90%  $N_2$ ) La<sub>1.</sub>  $_x$ Ca $_x$ MeO<sub>3- $\delta$ </sub> (Me=Fe, Mn) perovskites were used to clarify the effect of reaction medium. Data demonstrate the instability of x>0.3 perovskites in reaction medium very probably due to thermal evolution of oxygen from the samples causes segregation of the resulting oxygen vacancies, which is accompanied by formation of multiple planar defects in the perovskite structure and nanosized manganese oxide/iron oxides and calcium oxide particles on the surface. The same structural changes were revealed after heating in vacuum while heating in the air does not result in perovskite decomposition. Hence the main reason of perovskites (x≥0.3) decomposition under reaction medium is lower than in the air oxygen content.

O.S.B.7.

# THERMOCHEMICAL PROPERTIES OF ZIRCONIUM, MOLYBDENUM, VANADIUM AND CHROMIUM ALUMINIDES

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The values of formation heats, entropies and temperature dependences of heat capacities of zirconium, molybdenum, vanadium and chromium aluminides missed in the thermodynamic databases are given in the present paper. The computer modeling of smelting (by means of aluminothermic reduction of oxides) Zr-Al; Mo-Ti-Al; Mo-Ti-V-Cr-Al alloys has been performed using these values of thermochemical properties of aluminides with HSC Chemistry 6.1 software. The experimental smelting of above alloys was carried out by the out-of-furnace aluminothermic method. The validity of the model to the real process was shown by comparing calculation results with experimental data of smelting (chemical and phase composition).

O.S.B.8.

# THERMOCHEMICAL SYNTHESIS OF ALUMINIUM-VANADIUM-NITROGEN ALLOYS UNDER THE NITROGEN ATMOSPHERE

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In the present paper the possibility of thermochemical synthesis of V-Al-N alloys under the nitrogen at normal pressure has been considered. The nitridation processes of V-Al master alloys containing 50-75 wt-% of vanadium as well as the mixtures of those master alloys with  $V_2O_3$  and  $V_2O_5$  were investigated by the methods of differential thermal (NETZSCH STA 449 C Jupiter) and mass-spectrometric (QMS 403 C Aëolos) analysis. The samples were heated at various rates up to  $1500^{\circ}$ C. The paper includes data on the phase composition for the obtained alloys. Also, there is a dependence of their nitridation degree on the initial composition of master alloys, the presence of oxide additives and the heating rate. As a result of these investigations the possibility to obtain V-Al-N alloys with various compositions using the method of their direct nitridation at normal pressure has been established.

O.S.B.9.

# SYNERGETIC EFFECT IN THE LaFeO<sub>3</sub>-CeO<sub>2</sub> SYSTEM TOWARDS CATALYTIC ACTIVITY IN HIGH TEMPERATURE REACTIONS WITH OXYGEN PARTICIPATION

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Mechanochemical activation of blends of well-crystallized LaFeO $_3$  and CeO $_2$  (La : Ce = 0.05÷2) resulted in sharp increase of oxygen mobility in thus prepared perovskite-fluorite composites, as measured by  $^{16}\text{O}_2/^{18}\text{O}_2$  SSITKA at  $800^{0}\text{C}$ , in comparison with initial compounds. Although no formation of new phases was detected, deviation of the surface composition of mechanically activated samples from stoichiometric evidenced the development of the network of interphase boundaries that are responsible for fast oxygen transfer. It is increase of oxygen mobility that explains observed synergetic effect in perovskite-fluorite composites towards catalytic activity in the high-temperature (400÷900 $^{\circ}$ C) reactions with oxygen participation such as  $N_2$ O decomposition,  $NH_3$  and  $CH_4$  oxidation.

O.S.B.10.

# SIZE EFFECT UNDER PHORETIC COATINGS PREPARATION

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The problem of raising operation reliability and longevity of machinery and equipment that operate under the conditions of simultaneous action of aggressive media and high temperatures is of importance from the viewpoint of saving material resources and one of the most urgent problems in material science. Current material science is focused on science-based selection of materials for coatings and production of nanostructured coatings characterized by higher level of properties. In order to attain high adhesion characteristics for electrophoretic coatings, two steps of deposition process have been studied taking into account the particle size of initial powders. First the process conditions in deposition of electrophoretic coatings, in particular the effect of the molybdenum disilicide particle size (micro- and nanosized powders) on the process of deposition onto a molybdenum substrate were studied. Then the character of consolidation process and the structure of sintered in vacuum coatings were studied. In the case of microsized powders, the consolidation process at 1650 °C was established to proceed via a liquid phase sintering mechanism, whereas nanosized powders consolidate via a solid phase sintering only. Herein no marked increase in the particle size was observed. The possibility of changing properties of electrophoretic coatings by using combination of different layers prepared by deposition of micro- and nanosized powders was studied. The influence of impurities and intermediate products on the consolidation process as well as the data of electron-microscopic and metallographic analyses, microhardness distribution along the coating depth, its dependence on the coating deposition conditions and heat treatment have been discussed.

O.S.B.11.

# PHASE RELATIONS AND ADVANCED MATERIALS IN THE ${\bf ZrO_2(HfO_2)\text{-}Y_2O_3\text{-}Sm_2O_3}~SYSTEMS$

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The  $ZrO_2(HfO_2)-Y_2O_3-Sm_2O_3$  systems are of practical interest for creation engineering, optical, high-refractory materials, thermal barrier coatings, oxygen sensors, electroceramics and ones. These systems contains such phases like stabilized zirconia (hafnia) and yttria doped  $Sm_2Zr_2O_7$  ( $Sm_2Hf_2O_7$ ) which can be interesting candidates for the oxide ion conductor in fuel cells because their high thermodynamic stability and considerable ion conductivity at elevated temperatures.

Phase equilibria in the  $ZrO_2(HfO_2)-Y_2O_3-Sm_2O_3$  systems were studied in the temperature range 1100-2700 °C by both experimental methods (X-ray diffraction at 20 °C to determine phase contents, petrography and electron microprobe X-ray analysis) and theoretical means (development of a mathematical model for the liquidus surfaces by means of reduced polynomial methods).

Projections of the liquidus and solidus surfaces, isothermal sections at 1100, 1250, 1600 and 1900 °C were developed for the  $ZrO_2(HfO_2)-Y_2O_3-Sm_2O_3$  systems. The structure of bounding binary systems defined the phase equilibria in the ternary systems. No ternary compounds were found. The liquidus was characterized by the presence of two four-phase invariant equilibria. Ternary solid solution regions were determined based on constituent oxides: monoclinic (M), tetragonal (T), cubic with fluorite-type structure (F)  $ZrO_2(HfO_2)$ , hexagonal (A) and monoclinic (B)  $Sm_2O_3$ , cubic form of rare-earth oxides (C-type) and hexagonal (H)  $Y_2O_3$  as well as intermediate phases with pyrochlore type structure  $Sm_2Zr_2O_7$  ( $Sm_2Hf_2O_7$ , Py). The refined lattice parameters of the unit cells and the boundaries of the homogeneity fields for solid solutions were determined.

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O.S.B.12.

# MATERIAL BEHAVIOR AT THE PRE-FRACTURE STAGE AND A NEW METHOD FOR ESTIMATING THE PLASTICITY MARGIN OF MATERIALS WORKED BY PRESSING

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The behavior of various materials is addressed in the frame of auto-wave theory. The investigations were performed for pure metals as well as uni- and multi-phase alloys in single-crystal, polycrystalline and nanostructured state. The test samples were examined at the final stage of plastic deformation upon transition to viscous fracture. It is shown that under the above conditions collapse of the localized plasticity auto-wave would occur in the object under study no matter what its nature. The location of main crack and the instant of fracture can be determined from the quantitative characteristics of auto-wave collapse. It is found that on the base of such data plasticity margin can be determined for a material worked by cold forming operation.

PL.S.II.1.

# CHANGE IN THE CHEMICAL AND ELECTRONIC PROPERTIES OF OXIDE NANOPARTICLES BY SOLID STATE REACTIONS AT THE BOUNDARIES TO ORGANIC CRYSTALS

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Amongst challenges for obtaining various photonic nanomaterials, anion doping to the commercially available oxide nanoparticles is advantageous over syntheses from solution or gaseous phases, chiefly due to the preferential reaction at the near surface region, which most of the photonic functions are originated from. Solid state interfacial reactions under mechanical stressing without external heating or irradiation are appropriate for the purpose due to their relatively simple procedure, together with the affordability of mass production at a reasonable cost. Apparent drawbacks like contamination, agglomeration or crystallographical degradation could be minimized by choosing appropriate doping sources and combining with post annealing treatments. In the present overview, some solid state mechanochemical reactions at the boundaries between nanoparticles of TiO<sub>2</sub>, ZnO or Nb<sub>2</sub>O<sub>5</sub> and some organic crystals containing N and F, are examined by XRD, UV-Vis-NIR DRA, XPS, EDXS, MAS-NMR, or HRTEM. Mechanisms involved, i.e, oxidative decomposition of the organic ingredients, introduction of oxygen vacancies and ligand exchange, are elucidated. Comparison with the processes involving aqueous solutions will also be referred.

PL.S.II.2.

### INFRARED STUDY OF SOFT CONDENSED MATTER

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Infrared spectroscopy is a powerful technique in the study of condensed matter since the energy of electronic excitations and lattice vibrations fall in its range. It is very useful in the study of electronic correlations, electron-phonon interactions or some structural correlations. Very often these measurements need a broad spectral range and a high brilliance available at synchrotron light sources.

Several human diseases, ranging from Alzheimer's to prion disease, have now been identified to be caused by proteins which auto-assemble into high molecular weight aggregates. The force of infrared spectroscopy will be illustrated in the case of Huntingon's Disease (HD) and multiple sclerosis (MS).

There is a subgroup of ten diseases that are related to abnormal polyglutamine (polyQ) repeats, one of which is Huntingon's Disease (HD). Its symptoms are progressive deterioration of cognitive and motor functions, along with extensive loss of neurons primarily in the striatum. We used a rat model of HD to examine the chemical makeup of the brain slices. We have investigated the striatum with synchrotron-assisted Fourier transform infrared microspectroscopy (SIRMS). One brain hemisphere was infected with HD while keeping the second one as a control. The two types of matter in the striatum are affected in different manners: in neuron-rich gray matter exposed to the disease, a higher content of aggregated protein is detected as early as 6 weeks after infection, but no signs of cell death up to 8 weeks. In contrast, myelin-rich white matter does not show any aggregates, but surprisingly shows a significant increase in phosphorylation. We interpret this as the activation of the cellular response to stress which leads in the end to cell death.

The drastic changes in the white matter were detected in the case of multiple sclerosis (MS). We have studied its animal model, the experimental autoimmune encephalomyelitis (EAE). It is characterized by heavy loss of the insulating lipid-layer, the myelin around axons. This has been clearly confirmed by SIRMS and FTIR. Analysis of spatially resolved maps by both unsupervised principal component analysis and chemical signatures show additional features of this disease.

Both studies indicate that SIRMS is a powerful tool of detecting complex chemical processes in biological tissue in a relatively easy way.

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PL.S.II.3.

# DOPING, STRAINS AND ELECTRIC FIELD EFFECT ON SUPERCONDUCTIVITY IN ULTRA-THIN CUPRATE FILMS

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We summarize our main results of systematic experiments on strained cuprate films grown by laser ablation [1-3], and then discuss recent work (in close collaboration with Ivan Bozovic et al. from BNL) to smoothly tune the carrier concentration of MBE grown LSCO monolayer by means of an applied electric field [4,5]. Thin film devices were made in an electrical double layer transistor configuration utilizing an ionic liquid as gate electrolyte. Very large fields and induced changes in surface carrier density enable shifts in the critical temperature by up to 30 K. As reported elsewhere [4], numerous resistance vs temperature and carrier density curves were recorded and have shown to collapse onto a single function as predicted for a 2D superconductor-insulator transition. The observed critical resistance is precisely the quantum resistance for pairs,  $R_Q = h/(2e)^2 = 6.45 \text{ k}\Omega$ , suggestive of a phase transition driven by quantum phase fluctuations, and Cooper pair (de)localization. The implications of these results and ongoing field studies on other materials will also be discussed [5].

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PL.S.II.4.

# UNDERSTANDING THE MECHANISMS OF CARBON NANOTUBE GROWTH TERMINATION USING REAL TIME ENVIRONMENTAL TRANSMISSION ELECTRON MICROSCOPY

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Vertically aligned single-walled carbon nanotube (SWNT) carpets have received enormous attention, as they have a large number of potential applications. However, a lack of understanding of the mechanisms of growth termination remains a limiting factor in optimizing these structures for widespread usage. In order to better understand the growth termination phenomena, we have investigated the evolution of catalyst morphology using both standard and in-situ transmission electron microscopy techniques. A series of tightly controlled annealing and growth studies were performed in a dedicated chemical vapor deposition system using three different gas ambients (hydrogen, hydrogen and water and atomic hydrogen and water). Quantitative characterization of the catalyst sizes as a function of either annealing or growth time leads to an explanation for growth termination implicating both the processes of Ostwald ripening and iron diffusion into the substrate.[1] The presence of water vapor in the growth ambient is correlated with a decrease in both Ostwald ripening and iron diffusion rates.[2] Little correlation between the rates of growth termination and the relative carbon concentration was found, indicating that carbon overgrowth does not play a strong role in growth termination.[3] These results are corroborated by real time observations of nanotubes growth and termination in a dedicated environmental cell transmission electron microscope, where both ripening and substrate diffusion are directly observed. Finally, we have investigated the effect of substrate support on growth termination, and find that the particular stoichiometry of the alumina – as determined by the deposition method – can also strongly affect the growth outcomes.[4]

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PL.S.II.5.

# HIGH-K, HIGH-Q MICROWAVE DIELECTRICS: WHAT IS THE COMPROMISE TODAY?

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The development of a microwave dielectric material that would exhibit combination of a high dielectric constant and a high quality factor has been baffling the dielectric research community for decades. Most widespread ceramic microwave resonators with temperature stable resonant frequency are based on either complex perovskites with B-site cation ordering that exhibit very high quality factors (Qxf > 100000 GHz) and dielectric constant of K  $\approx$  30, or on tungsten-bronze-type 114 solid solutions that exhibit K between 70 and 90 with Oxf values not exceeding 11000 GHz. A successful compromise between the two groups of materials is represented by CaTiO<sub>3</sub> – REAlO<sub>3</sub> (RE = La, Nd) perovskite ceramics that combine a relatively high dielectric constant K > 40 and a high quality factor Qxf > 40000 GHz. Recently a new demand for miniaturization has emerged which presents a need for a material that would exhibit dielectric constant of at least 64 and quality factor above 15000 GHz with a temperature coefficient of resonant frequency within  $\pm$  10 ppm/K. The closest of the known materials to the required combination of properties are solid solutions based on incipient ferroelectric perovskites CaTiO<sub>3</sub> and SrTiO<sub>3</sub>. Unfortunately, however, the temperature coefficient of compositions with dielectric constants above 50, is far to high for most applications. In the contribution our approach towards such a material, based on two-phase ceramics with compositions in the vicinity of  $Ba_{6-3x}(Sm,Nd)_{8+2x}Ti_{18}O_{54}$  will be presented.

PL.S.II.6.

# KINETICS OF HIGH-TEMPERATURE SPREADING

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This presentation reviews the recent advances in the experimental and theoretical analysis of the high-temperature spreading of molten metals and oxides. In particular, it will review recent experiments based on the high-speed video recording of spontaneous spreading and compare the results with molecular dynamic simulations. The recorded spreading kinetics are compared with existing theories developed for room-temperature liquids. These results outline the critical role of the local dissipation at the triple solid-liquid-vapor junction in spreading at high-temperature and in how friction relates to atomic ordering in the liquid close to the interface.

PL.S.II.7.

# MATERIALS TRANSPORT AND CRYSTALLIZATION DURING THE AI INDUCED LAYER EXCHANGE (ALILE) PROCESS

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The ALILE process enables fabrication of thin polycrystalline Si films at relatively low temperature (< 450°C) making it highly promising for applications in thin film photovoltaics. While the driving forces for the metal-induced crystallization are rather well understood the details of the materials transport during the layer exchange are largely unknown. In this work the microstructure of stacks of a-Si(100nm)/Al(50nm)/Quartz, annealed at 450°C, has been investigated at different length scales by combining optical microscopy, analytical SEM and analytical TEM [1]. The results indicate that the ALILE and crystallization reaction proceeds by forming 20-50µm wide dendritic "cells" with Al deficient centers. Excessive upward transport of Al by epitaxial growth out of the existing Al grains into the a-Si was observed in a rim of about 10 µm width around the cells and to a smaller extent even a few tens of micrometers away from the reaction front. Using in-situ TEM the lateral and vertical transport of Al at the expanding crystallization front could be directly visualized for the first time. We propose that Coble-type diffusion of Al along the Al grain boundaries and/or the Al/a-Si interface, driven by the compressive stress in the Al layer, is responsible for the massive long range lateral and vertical transport of Al. Our findings shed new light on the redistribution of Al and Si during the ALILE process.

[1] B. Birajdar, T. Antesberger, M. Stutzmann, E. Spiecker, physica status solidi (RRL) 5, 172-174 (2011)

PL.S.II.8.

# NUCLEATION AND GROWTH OF COLLOIDAL NANOPARTICLES STUDIED BY COUPLED IN-SITU SPECTROSCOPIC METHODS

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Nanoparticles are among the most intensely studied nanoscale materials nowadays, yet a coherent mechanistic explanation for the evolution of particles during their chemical synthesis has not been provided so far in many cases. A decisive factor for such limited understanding rests in the fact that relevant data have often been obtained by ex-situ analytical methods requiring sample preparation techniques (SEM, TEM, XRD). The present talk shows that the essential time-resolved information on chemical and morphological state of reactants and particles can be obtained directly and in-situ via coupled XANES and SAXS analysis. From the obtained data, mechanism and kinetics of nanoparticle formation can be deduced. In consequence, improved particle synthesis strategies are derived that enable precise particle size control. The proposed strategy will be illustrated for different synthesis routes of colloidal noble-metal nanoparticles.

O.S.C.I.1.

# STRUCTURE, MAGNETISM AND ELECTRONIC PROPERTIES OF NANOCRYSTALLINE 3d-METALS ENCAPSULATED IN CARBON

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The most important problem from the point of view synthesis, investigation and application of nanocrystalline materials (mainly metals) is how one can provide the long-term stability of metastable materials and the same time to preserve the unique physical and chemical properties. This problem is not crucial when you have dealt with carbon-contained materials such as carbon nanotube, fullerene, graphene and so on. In the case of metallic materials in a nanocrystalline state there is a very serious protection problem. One variant is to solve this problem creating the "core-shell" structure, such as, for instance, magnetic metals (Me=Fe, Co, Ni and others) in a nanocrystalline state covered by carbon as a stable platform for multimodal purposes. Unfortunately, the detailed and systematic investigations of the above-mentioned materials are very little in spite of the attractive properties for different applications. There is also a lack of fundamental investigations of structure, magnetic and electronic properties for this kind of "core-shell" materials in a nanoscale range. In the given work the nanocomposites on the base of 3d-metals (Fe, Ni, Co, Fe-Co) covered by thin layers of carbon (Me@C) and having the average size less than 10 nm including carbon coating were synthesized by gas-condensation method. Structural parameters and electronic properties of metal-carbon nanocomposites have been studied by X-ray diffraction analysis, high resolution transmission electron microscopy, XPS, XAS, Raman and Mossbauer spectroscopy methods. It was found that carbon coating protects the metallic nanoparticles from the environmental degradation by providing a strong barrier against oxidation and ensure stability of the chemical and physical properties at least more than 1 year. Nanocomposites (Fe@C, Ni@C) demonstrate a novel catalyst mechanism with high catalytic activity and selectivity in the chlorobenzene transformations.

It was shown that the specific magnetization of iron and nickel encapsulated in carbon taking into account the content of carbon coating and carbides is turned out too abnormally small as compared with the one of bulk state. At the same time a magnetization of Co@C and alloy (Fe,Co)@C nanocomposites corresponds to the magnetization of bulk state of cobalt and Fe-Co alloy considering the carbon contribution as well. The unusual magnetic properties of Fe, Ni encapsulated in carbon in the nanoscale range will be discussed in the model of non-collinear magnetic structure for surface spins of metallic core.

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# THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

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O.S.C.I.2.

# SILICON NANOWIRE COATED MICROPARTICLES AS ADHESIVE DRUG DELIVERY DEVICES

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Materials science provides a vital impetus for the design of advanced medical vehicles for controlled drug delivery. Satisfactory adhesion of these devices onto biological surfaces is of great importance to achieve effective and targeted drug release over a prolonged period. Novel composite particles made by growing nanoscopic silicon wires from the surface of silica beads were tested in this study for their ability to affect permeability of an epithelial cell layer to various model drug compounds. Polyethylene glycol (PEG) is known to sterically stabilize particles and prevent binding of plasma protein; as such, it is a routine way to impart in vivo longevity to drug carriers. The effect of the particles in both their PEGylated and non-PEGylated forms on the disruption of the tight junctions in Caco-2 cells was also evaluated by means of: (a) confocal immunofluorescence microscopic analysis of zonula occludens-1 and f-actin; (b) measurements of trans-epithelial electrical resistance; and (c) real-time polymerase chain reaction analysis of the expression of PKC-α and PKC-Z, which regulate the fluidity of cell membranes, and RhoA and Rac1, which are involved in cell migration processes.

O.S.C.I.3.

# A HIGH-TEMPERATURE OPTIAL STUDY OF DEFECTS AND DIFFUSION IN LITHIUM DEFICIENT LITHIUM NIOBATE

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Under reducing conditions, optical spectra of lithium niobate, LiNbO<sub>3</sub> (LN), are dominated by broad electronic absorption bands in the visible and NIR region which have been attributed primarily to absorption due to various types of small polarons, see the recent review by Volk and Wöhleke [1]. The present high-temperature study at 1000°C reports on the oxygen activity, aO<sub>2</sub>, dependence of electronic absorption in lithium deficient LN (48.4 mol Li<sub>2</sub>O, c-LN). Absorption intensity is found to obey a power law of the form  $(aO_2)^m$  with  $m \approx -1/4$  which can be attributed to free small polarons [2]. The kinetics of redox processes in c-LN have been studied in aO2-jump experiments with sudden changes in aO2 under in-situ conditions. From the experiments, the chemical diffusion coefficient of c-LN has been determined as well as the diffusion coefficients of lithium vacancies and lithium ions at 1000°C [2].

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- [2] J. Shi, H. Fritze, G. Borchardt, K. -D. Becker, Phys. Chem. Chem. Phys. 2011, 13, 6925

O.S.C.I.4.

# (IN)COMMENSURABILITY OF CARBON NANOTUBES

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Unlike in planar graphene, nearest naighbors in simply rolled up graphene sheet, forming thus a nanotube, are not at the same distances. Consequently, the strain arises, being only partially compensated by relaxing procedure. Actually, there is one degree of freedom which cannot be numerically relaxed: torsion. A small torsion enlarges unit cell so much that the number of atoms within it overwhelms capabilities of conventional numerical codes. Moreover, there is no guarantee that single-wall carbon nanotube should be commensurate whatsoever.

Helical transformation with continual parameters of translational length and rotational angle (which correspond to elongation and torsion, respectively) pertains to the line group symmetry. By enabling analytical optimization of these parameters within a simple geometrical model and afterwards, by using numerical fully symmetry implemented method we confirm possible incommensurability of chiral carbon nanotubes.

O.S.C.I.5.

### PROPERTIES OF HELICALLY COILED NANOTUBES

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Carbon nanotube transforms to a helically coiled nanotube by regular substitution some of the carbon hexagons by pentagons (introducing thus positive Gaussian curvature) and heptagons (where negative curvature arises). Here we study stability and properties of regularly coiled single-wall carbon nanotubes using method of topological coordinates. Electronic bands and optical response functions are evaluated by means of line group symmetry adopted density functional tight binding implemented into the POLSym code.

O.S.C.I.6.

# THE PUZZLE-INTERLAYER MODEL: A UNIVERSAL APPROACH IN MATERIALS SCIENCE FOR DESCRIBING POROUS MATERIALS

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A porous material (pores and walls) of a certain porosity is an idealized two-phase system. The shape of the pore phase 1 is defined by a wall-phase 2. It is advantageous to analyse such samples by scattering experiments (i.e. Small-Angle Scattering, SAS). This technique excludes any destruction of the sample as a result of preparation processes. However, this technique requires geometric-beforehand-models.

By shifting the pieces of a three-dimensional puzzle a bit, an interlayer (wall-phase 2) between the pieces results. Now, chord length distributions (CLDs) are applied: the CLD of the interlayer and the CLD of the pores. The porosity results in terms of the mean chord lengths (Rosiwal, 1898). By use of the technique of Fourier transformation, SAS intensities can be interpreted in terms of both CLDs. This is illustrated for selected porous materials in detail.

O.S.C.I.7.

# MODEL OF "IN-SITU TENSILE TEST IN SEM" OF Al-Al<sub>4</sub>C<sub>3</sub> NANOMATERIALS

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The method of "in-situ tensile testing in SEM" is suitable for investigations of fracture mechanisms because it enables to observe and document deformation processes directly, thank to which the initiation and development of plastic deformation and fracture can be reliably described. The aim of the study was to evaluate the influence of selected volume fraction of Al<sub>4</sub>C<sub>3</sub> (4 vol.%) and Al<sub>2</sub>O<sub>3</sub> (1 vol.%) particles on the fracture mechanism by means of the method "in situ tensile test in SEM". The dispersion strengthened alloys Al-Al<sub>4</sub>C<sub>3</sub> manufactured by mechanical alloying using powder metallurgy technology are promising structural materials. One material of such type with 4 vol.% Al<sub>4</sub>C<sub>3</sub> was transformed by the ECAP method in two passes into a nanocomposite material. The experimental material was pressed through two right angled (90°) channels of a special die by route "C". The ECAP technology allows obtaining the very fine grained microstructure - nanostructure by multiple pressings through the die. According to the microstructure observations, the particles in our materials can be divided into three distinctive groups: A - small Al<sub>4</sub>C<sub>3</sub> particles, identified by TEM, with mean size approximately 30 nm which made up to 70% of the dispersoid volume fraction; B – large Al<sub>4</sub>C<sub>3</sub> particles with mean size between 1 and 2 µm, identified by scanning electron microscopy and on metallographic micrographs; and C - large Al<sub>2</sub>O<sub>3</sub> particles with mean size of 1 µm, found on metallographic micrographs and identified by scanning electron microscopy. Morphologically, Al<sub>4</sub>C<sub>3</sub> particles are elongated and Al<sub>2</sub>O<sub>3</sub> particles are spherical. Let us assume that particles of all categories during the high plastic deformation are distributed in rows. The mean size of grains before ECAP was 0.85 m. After ECAP occurs decreasing of mean grains size 200-300 nm. It has been shown that the deformation process causes break-up of large Al<sub>4</sub>C<sub>3</sub> particles and decohesion of smaller ones. Based on the microstructure changes observed in the process of deformation, the following model of fracture mechanism is proposed: the microstructure in the initial state is characterized by Al<sub>4</sub>C<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub> particles, categorized as A, B and C, whose geometric parameters depends on their volume fraction; with increasing tensile load local cracks, predominantly on specimen side surfaces, are formed by rupture of large (B) and decohesion of smaller (C and/or A) particles; in further increasing deformation of nanocomposite materials the nanograin boundaries start to play an important role. The final rupture, i.e. interconnection of the side cracks along the loading direction, takes place at nanograin boundaries.

O.S.C.I.8.

# SOLVOTHERMAL SYNTHESIS OF NEW 2D LAYERED NANOCRYSTALLINE INORGANIC-ORGANIC HYBRID V<sub>4</sub>O<sub>4</sub>(OH)<sub>2</sub>(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>)·DMF COMPOUND AND ITS MAGNETIC PROPERTIES

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The title compound has been synthesized under solvothermal conditions by reacting vanadium(V) oxytriisopropoxide with terephthalic acid in N,N-dimethylformamide. A combination of synchrotron powder diffraction, infrared spectroscopy, scanning and transmission electron microscopy, thermal and chemical analysis elucidated the chemical, structural and microstructural features of new 2D layered inorganic-organic framework. Due to the low-crystallinity of the final material, its crystal structure has been solved from synchrotron X-ray powder diffraction data using a direct space global optimization technique and subsequent constraint Rietveld refinement. [V<sub>4</sub>O<sub>4</sub>(OH)<sub>2</sub>(O<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>)·DMF] crystallizes in the monoclinic system (space group P2/m (No. 10)); cell parameters: a = 20.923(4), b = 5.963(4), c =20.425(3) Å,  $\beta = 123.701(6)$  °, V = 2120.1(15) Å<sup>3</sup>, Z = 2,  $D_C = 1.613(1)$  g/cm<sup>3</sup>. The overall structure can be described as an array of parallel 2D layers running along [-101] direction, consisting of two types of vanadium oxidation states and coordination polyhedra; face-shared trigonal prisms (V<sup>4+</sup>) and distorted corner-shared square pyramids (V<sup>5+</sup>). Both configurations form independent parallel chains oriented along the 2-fold symmetry crystallographic b-axis mutually interlinked with terephthalate ligands in a monodentate mode perpendicular to it. The structural cohesion has been achieved by interlayer C-H···O hydrogen bonding via N.Ndimethylformamide molecule. The morphology of the compound exhibits long nanofibers, with the growth direction along the layered [-101] axis. The magnetic susceptibility measurements show that the magnetic properties of  $V_4O_4(OH)_2(O_2CC_6H_4CO_2)$ ·DMF can be described by a linear antiferromagnetic chain model, with the isotropic exchange interaction of J = -75 K between the nearest  $V^{4+}$  neighbours of S = 1/2.

O.S.C.I.9.

# COMPOSITION – PROPERTIES RELATIONSHIP OF NANOSTRUCTURED POLYCARBONATE-BASED POLYURETHANE/ NANOCOMPOSITES

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Novel polycarbonate based polyurethane elastomers (PC-PU) as well as their nanocomposites with organic-modified clay (Bentonite for organic systems) with improved mechanical, thermomechanical and thermal properties were synthesized and characterized. Hard segments, which provide physical crosslinks by intermolecular association through hydrogen bonding, mainly composed of hexamethylene diisocyanate butane-1,4-diol (BD) as a chain extender. As a source of soft segments, selected aliphatic polycarbonate diols with molecular weight around 2000 (T5652, T4672, T4692) differing in constitution of the polycarbonate chains as well as dibutyltin dilaurate as a catalyst were used. The dispersion of nanofiller was achieved by one day swelling in macrodiol and butanediol mixture and a brief mixing before addition of isocyanate component. The samples with different hard segment content were prepared in the form of sheets and films using a one-step procedure. Ratio was constant and R was varied from 0.3  $(r = [NCO]/[OH]_{Total} = 1.05$  and  $R = [OH]_{MD}/[OH]_{RD}$ ). One series was synthesized without chain extander. The procedure for film preparation was the same, only the final mixture was spread on polypropylene sheets instead of putting into the Teflon molds. The influence of hard segment content as well as nanofiller, macrodiol, chain extander and diisocyanate type on mechanical, thermomechanical, thermal, surface and transport properties was examined. For the surface topography characterization, as well as for internal arrangement and microphase separation of PU's on nanometer/micrometer scale (analysis of broken area of PU sheets), atomic force microscopy (AFM) was used. Very high elongation at break together with high tensile strength lead to very high toughness values compared to polyether or polyester based PU's, Such a good properties seem to be a result of a distinct segmentation of this material on submicron to nanometer scale, with the hard domains acting as physical crosslinks through hydrogen bonding.

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O.S.C.I.10.

# FEATURES OF THE NANOSTRUCTURED MATERIALS FOR NONLINEAR OPTICS AND SOLAR ENERGY APPLICATIONS

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The nonlinear refraction and third order susceptibility are discussed for different organic materials doped with fullerenes, shungites, carbon nanotubes, carbon nanofibers, quantum dots, etc. nanoobjects. The evidence of the correlation between laser induced change of the refractive index and charge carrier mobility are obtained. The features of new nanocomposites for their possible optoelectronics, laser techniques and solar energy applications are considered. The results have been supported by RFBR grant #10-03-00916.

O.S.C.I.11.

# PREPARATION OF METAL NANOPARTICLES FOR SOFC ANODES USING SONOELECTROCHEMICAL METHODS

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The aim of this research is the preparation of stable water suspensions of metallic nanoparticles, such us gold, silver and copper by an ultrasound assisted electrochemical process. The obtained metallic nanoparticles are going to be used to improve durability and efficiency of SOFC anode cermets against degradation phenomena arising from carbon and sulfur containing compounds in the feed. The particles are stabilized in order to prevent agglomeration. Formation and size of the nanoparticles are affected by parameters like current density, current pulse duration and ultrasonic pulse duration. The optimization of the size of the metal nanoparticles and of the efficiency of the sonoelectrochemical procedure was succeeded by varying these parameters both in galvanostatic as well as potentiostatic conditions. The obtained nanoparticles were characterized by DLS and TEM.

O.S.C.I.12.

# SINTERABILITY EVALUATION OF ALUMINUM METAL MATRIX COMPOSITES POWDER WITH DIFFERENT CHEMICAL COMPOSTITIONS

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Recently, research in lightweight materials has been improved significantly. Aluminum metal matrix composites powder offer high mechanical properties, low coefficient of thermal expansion and good weight strength ratio. In this research, we analyzed Aluminum alloy powders with different chemical composition, Al-Si-Cu-Mg and Al-Si-Fe-Mg. SiC particulate strengthening also was added to improve its mechanical properties. Powders were compacted up to 700 MPa with dual action press. Green density increased with increasing compaction pressure. All the compacted powders were sintered under flowing ultra high purity nitrogen gas. Modification in sintering variables was done to determine optimum sintering conditions. Sintered density increased with increasing sintering temperature up to 560 C. Reaction during sintering and chemical composition of powder played important role on sintered properties of aluminum powder. T6 heat treatment was carried out to produce fine precipitates to impede movement of dislocation to increase their mechanical properties. The chemical composition of this materials allow for the potential formation of several strengthening precipitates including  $\theta$ (Al<sub>2</sub>Cu) and β (Mg<sub>2</sub>Si). The heat treatment involved solutionizing materials followed by water quenching, and artificially aging. Optical Microscopy, SEM and X-Ray Diffraction were used to characterize materials. And DSC-TGA was also used to determine thermal properties of these powders.

Keywords: Aluminum Powder, Sintering, Heat Treatment, Mechanical Properties.

O.S.C.I.13.

# DISPERSION STATE, OPTICAL CHARACTERIZATION AND ELECTRICAL PROPERTIES OF CARBON NANOTUBE / POLYMER COMPOSITES

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With intrinsic electrical conductivities ranging from  $10^4$  to  $10^7$  S.m<sup>-1</sup>, carbon nanotubes (CNT) represent one of the most stirring up additives for designing highly-conductive polymer composites. For such systems, Nan's law predicts percolation thresholds for CNT volume fractions around 0,1%.

However, several CNT percent are practically needed. Morever, recent literature reviews show a very large scatter within the data ranges between 10<sup>-5</sup> to 10<sup>2</sup> S.m<sup>-1</sup>, orders of magnitude less conducting than the corresponding nanoparticles. Based on new optical microscopy approach, this contribution will try and shed some light on the reasons for such discrepancies. Routes to minimize gaps between theory and experiments will then be discussed.

O.S.C.I.14.

### REACTIVITY OF NANOCRYSTALLINE MAGNESIUM

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Magnesium and magnesium-based alloys are regarded as perspective materials for hydrogen storage due to high theoretical hydrogen capacity of magnesium, relatively low cost and abundance of the raw materials. However, slow kinetics of hydrogen absorption/desorption and high temperature of MgH<sub>2</sub> decomposition stimulated a large number of researches directed to overcome these drawbacks. The recent results of the investigations have shown that fabrication of nanocrystalline magnesium-catalyst composites greatly improve hydriding properties of magnesium. At the same time some peculiarities in hydriding properties of nanocrystalline magnesium (such as "hysteresis" phenomenon, unusual shape of kinetic curves, very strong dependence of reaction rate on hydrogen pressure and incomplete transformation into hydride) have been observed by many authors. In this work the role of nucleation processes in reactivity of magnesium toward hydrogen is discussed. It has been shown that observed peculiarities can be explained by hampered hydride nucleation in nanocrystalline magnesium and this should be taken into consideration at investigation and development of nanocrystalline hydrogen storage materials.

O.S.C.II.1.

# 3D NANOSTRUCTURED OXIDES MATERIALS GROWN AT THE SURFACE OF LIQUID METALLIC ALLOYS

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The oxidation of some liquid-metal alloys under the certain environment results in the formation of porous or 3D nanostructured oxides. In particular, the oxidation of Hg, Ga or Bi melts, containing small amount of Al, allows synthesizing a porous monoliths of nanostructured oxyhydroxide of alumina (NOA) [1]. The structure, physical and chemical properties of NOA materials synthesized at Hg or Ga alloys surface in a humid air or gas are the most studied. Typical growth rate of NOA monoliths in a humid air is about 1 cm/hour at the temperatures 25 - 30 °C. Using of the different alloys provides quite similar results and the properties of NOA materials: small density (0,02 – 0,04 gm/cm<sup>3</sup>), high porosity (99 %vol.), large specific surface ~300 m<sup>2</sup>/gm. The structure of NOA consist of the three-dimensional network of the amorphous nanofibrils (5 - 7 nm in diameter and 120 - 150 nm in length) with chemical composition ~ Al<sub>2</sub>O<sub>3</sub>·3,6H<sub>2</sub>O. An annealing in the temperature range 900 – 1700 °C does not destroy solidity and porous structure of NOA samples, but the linear sizes of the samples are decreasing proportionally, the density increase from 0,02 up to 3 g/cm<sup>3</sup>; the porosity and specific surface decreases: 99.3 - 25 % and 300 - 1 m<sup>2</sup>/g respectively. All these transformations accompanied by structural and phase transitions: starting from the supramolecular to amorphous states and from amorphous to the crystalline  $\gamma - \theta$  - and  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>.

TGA, IR, XRD and TEM techniques was applied for the studies of the products of Al selective oxidation at the surface of Hg and Ga melts. Chemical composition of NOA materials, kinetics of the evolution of 3D structure was also studied in the temperature range 25 - 1700 °C. Obtained results allowed us to propose a quantitative model of 3D structure of porous monolithic nanocomposites and simulate the evolution of its density, porosity and specific surface in a wide temperature range. Properties of some composite 3D structures (e.g. NOA – SiO<sub>2</sub>, NOA – TiO<sub>2</sub>, NOA – Ni) also can be described in the frames of the model proposed.

 T. di Costanzo, A.A. Fomkin, C. Frappart, A.N. Khodan, D.G. Kuznetsov et al. Materials Science Forum Vols. 453-454 (2004) pp. 315-322

O.S.C.II.2.

# STRUCTURE EVOLUTION AT HEATING OF FINEMET TYPE AMORPHOUS MICROWIRES

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Structure evolution during heating of FINEMET type amorphous microwire was investigated using differential scanning calorimetry, X-ray diffraction and tomographic atom probe. It was shown that differential scanning calorimetry is a suitable technique for precision investigation of relaxation process in samples under investigations. Relaxation of atomic structure of amorphous phase at annealing was accompanied by increase of its Curie point, which was determined as a temperature of heat capacity peak on calorimetric curve at continuous heating. Annealing temperature dependencies of Curie point shows that relaxation process continuously passes into nanocrystallization of amorphous alloys. Tomographic atom probe method was used to investigate changes in amorphous phase structure at relaxation. These investigations show redistribution of components in amorphous phase during annealing. This was associated with clustering inside the amorphous phase, its separation into two phases with different chemical compositions. At that precipitation of α-Fe nanocrystalline nuclei in amorphous phase at further annealing was associated with disappearance of iron-rich type of clusters. Apparent values of activation energy of relaxation were evaluated from the data of differential scanning calorimetry. Comparison of the obtained results with the data for ribbon FINEMET type allows allows us to propose that glass coating of microwires has nearly no effect on the nanocrystallization process in amorphous alloys. This work is supported in the frame of federal target program «Scientific and scientific-pedagogical personnel of innovative Russia», state contract P1025.

O.S.C.II.3.

# SYNTHESIS AND INVESTIGATIONS OF STRUCTURE AND ELECTROCHEMICAL PROPERTIES OF PtCr/ EBONEX CATALYSTS FOR PEM WATER ELECTROLYSIS

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The proton exchange membrane water electrolysis (PEMWE) has attracted huge interest in the recent years as method for production of hydrogen with high purity offering several advantages over the traditional technologies - no usage of liquid electrolyte, lower energy parasitic losses, higher current densities, etc. The anodic reaction of oxygen evolution (OER) is of particular research interest since it is the main source of energy losses and electrode degradation problems. The preparation technique of the catalyst and the type of the supporting material used are very important for the efficiently of the PEMWE. In this work combinations of mono- and bimetallic composite ORR catalysts in which Pt is partly or totally replaced by Cr in different ratios were synthesised from acetilacetonate precursors (M[(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>n</sub>]<sub>m</sub> or M-acac, M=Pt, Cr) using the sol-gel method. The selected compositions were chosen after preliminary theoretical calculations and considerations based on the Brewer interactive bonding theory and corresponding predictions about the probability for hyper- hypo-d-electron effects. A nonstoichiometric Magneli phase titanium oxide (Ti<sub>n</sub>O<sub>2n-1</sub>) known under the registered trade name Ebonex (Atraverda Inc, UK) was used as catalytic support. This material possesses unique combination of excellent electrical conductivity approaching that of a metal and high corrosion resistance. It was applied as a substitute of the conventional carbon catalytic supports. In order to achieve higher surface area the as-received Ebonex was subjected to mechanical treatment in a planetary ball mill. The morphology and structure of the synthesized composites were studied by SEM, XRD and XPS. The electrocatalytic properties were investigated using the electrochemical techniques of cyclic voltammetry and steady state polarization. The investigations showed that no alloying between Pt and Cr occurs, while Cr is in amorphous oxidized state. In order to evaluate the electrode area accessible for the electrochemical reaction and thus to assess the utilisation of the catalysts, the morphology factor has been determined. The results showed that Pt/Cr/Ebonex facilitates the oxygen evolution which starts at lower overpotential and proceeds with higher rate compared to the monometallic Pt/Ebonex and Cr/Ebonex catalysts. The improved activity was explained with hypo-hyper-d-electron interactions between Pt and Cr and synergism with the Ebonex support, proven by XPS analysis.

O.S.C.II.4.

# MORPHOLOGY OF COMPOSITE INORGANIC MATRIX CONTAINING ION-EXCHANGER NANOPARTICLES

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The aim of the work was to elucidate a nature of charge-selective properties of macroporous composite inorganic membranes modified with nanoparticles of hydrated zirconium dioxide (HZD). These membranes have been found to be selective towards cations in alkaline media, at the same time they demonstrate anion-exchange properties in acidic media. The composite membranes show charge selectivity in the field of solution concentration, which does not provide overlapping of intraporous diffusion constituents of electric double layer. The membranes have been investigating using a number of methods, namely standard contact porometry, potentiometry and scanning electron microscopy. The method of transmission electron microscopy was used to research individual HZD as well as ceramic powder, which had been obtained by crumbling up of the non-modified matrix.

Differential curves of volume and surface distribution have been factorized using Lorentz functions, each maximum has been related to either structure element both of the matrix and the ion-exchanger. Calculations according to homogeneous and heterogeneous geometrical models were used for this purpose. It has been found that the insertion of HZD nanoparticles into the matrix pores results in formation of micropores as well as additional mesopores, the radius of which  $(r_n)$  is not higher than 13÷25 nm. A structure of the ceramic matrix has been shown to be formed with particles of micron size. Some aggregates of smaller particles are localized episodically on the surface of larger particles. A size of globular particles of the ion-exchanger  $(r_n=3 \div 5 \text{ nm})$  and their packing (cubic body-centered ore simple cubic) are depended on a number of modification cycle: more friable structure have been found for the membranes with higher content of HZD. The nanoparticles form aggregates ( $r_p=20\div23$  nm), which are not only deposited on the walls of the matrix pores, but also cork up them. The potentiometric measurements followed by modelling of transport number through the membranes have been carried out. The  $r_p$  value was used as a simulation parameter. It was shown that the pores, which determine charge selectivity, are formed due to corking of the matrix macropores with aggregates of HZD nanoparticles. Maximal size of these pores is 13÷25 nm, this is in agreement with porometric data.

The results obtained from porometric and potentiometric measurements have been confirmed with electron microscopy. As for individual components, two types of particles have been recognized. In the case of composite membranes large channels of micron size are visible, though nanosized pores between them cannot be diagnosed using both scanning and transmission microscopy. Thus the combination of porometry and potentiomety gives information about structure of composite membranes especially in the case of a small content of ion-exchangers in ceramic matrix. Influence of morphology on functional properties of the membranes is considered. These properties are intermediate between those for ion-exchange polymer membranes and inert diaphragms.

O.S.C.II.5.

# SYNTHESIS OF NICKEL FERRITE NANOPARTICLES BY THE CRUCIBLE-FREE AEROSOL TECHNIQUE

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Nickel ferrite nanoparticles (5-50 nm in sizes) were prepared via the crucible-free aerosol technique. Pure Ni and Fe wired metals were HF co-evaporated in helium gas flow accompanied by the split oxidation process. Due to the vapor condensation some ferrite nanoparticles were obtained. They had a well-defined shape and little change in sizes and were characterized by SEM, EDX, XRD, BET and VSM. The best regimes for the synthesis of nanoferrites with given average sizes and desired phase composition were determined. DC electric field (up to 6 kV/cm) applied during the synthesis essentially changes the main magnetic properties of the nanoparticles. This multiferroic material was tested as gas sensor and electromagnetic field detector and number of unusual properties were discovered.

O.S.C.II.6.

### HYDROGEN STATE IN MECHANICALLY PREPARED TI/B NANOCOMPOSITE

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Evolution in hydrogen state interrelated with morphological, structural and chemical evolution of ball-milled Ti/B was studied in detail as a function of mechanical treatment. Ti/B powder continuously changes both in composition and morphology during ball-milling in H<sub>2</sub> flow: The powder composition varies from Ti/B to TiH<sub>2-x</sub>/B causing a change in mechanical properties. The role of boron additive also changes from preventing the Ti particles from sticking together in the early stages to a matrix material participating in Ti - B interface reactions in the intermediate and final stages of the process. Boron atoms participating in the formation of nanoscopic holes gave rise to new H states in the hydride by changing the local atomic state of Ti atoms. The dynamics of the formation of these sites and the redistribution of hydrogen between different types of occupation sites in dependence of phase composition and milling time of the powders are also studied. As was shown, hydrogen is situated at interstitial positions in Ti characterized by high thermal stability,  $T_{max} = 946 - 1000$  K on early stages of intermixing of Ti and B powders. Transformation of Ti/TiH<sub>2.x</sub>/B to a nanocomposite consisting of a boron matrix with embedded Ti and TiH2-x nanofragments is accompanied by two new desorption peaks emerge, at  $T_{max} = 850$  K and  $T_{max} = 750 - 800$  K. Finally, a new lowtemperature peak emerges at  $T_{max} = 600 - 650$  K, which is the result of boron interaction with the powders: appearance of nanosized pores that contain weakly bound hydrogen, and boron introduction into the TiH2-x lattice, where it modifies the bonding structure of Ti, hereby lowering the binding energy of hydrogen in the hydride.

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O.S.C.II.7.

# MECHANICAL PROPERTIES OF RARE-EARTH DOPED $\mathrm{Si}_3\mathrm{N}_4$ AND $\mathrm{Si}_3\mathrm{N}_4/\mathrm{SiC}$ CERAMICS

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The influence of rare-earth oxide additives (La2O3, Y2O3, Yb2O3 and Lu2O3) on the microstructure and mechanical properties of hot-pressed silicon nitride and Si3N4 + SiC nanocomposites have been investigated. The composites exhibited finer microstructure compared to monolithic materials and the aspect ratio of the Si3N4 grains increased with decreasing ionic radius of rare-earth elements both in monolithic Si3N4 and in Si3N4+SiC nanocomposites. Chevron Notched Beam technique and four-point bending mode have been used for fracture toughness and strength measurements, respectively. The hardness of both kinds of material increased with decreasing ionic radius of rare-earth element. The fracture toughness of monoliths was higher due to the coarser microstructures and due to more toughening mechanisms during the crack propagation. Materials with higher aspect ratio of the Si3N4 grains (Lu or Yb additives) exhibited crack deflection more frequently compared to the Si3N4 doped with La or Y, which was responsible for the higher fracture toughness. The bending strength slightly increased with decreasing ionic radius of rare-earth element. The positive influence of finer microstructure of the composites on the strength was not observed because of the present strength degrading defects.

O.S.C.II.8.

# CHEMISTRY AND MOCVD APPLICATIONS OF VOLATILE DIMETHYLGOLD(III) COMPOUNDS WITH (O,N,S)-DONOR LIGANDS

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Thin Au films and nanomaterials find wide applications in optical devices, catalysis, solar cells, decorative and restoration technologies. MOCVD technique is one of the methods for depositing such materials. Chemistry of precursors is very important for realization of Au deposition processes. Now Au CVD precursor application is limited because of small choice of volatile Au compounds. Volatile dimethylgold(III) complexes were synthesized in this work. The new approaches to synthesis of precursors were offered. Carboxylate, salicylaldiminate, quinolinate derivatives were used as chelating agents. Different physicochemical methods were applied for characterization and studying of compounds: IR-, NMR-spectroscopy, mass spectrometry, element analysis, melting points, X-ray single structure analysis. Thermal properties in solid state were investigated by means of DTA/TG method, qualitative volatility rows of vaporization processes were determined. The temperature dependences of saturated vapor pressure were measured by means of effusion Knudsen's method, and standard thermodynamic parameters of sublimation process  $\Delta H_T$  and  $\Delta S_T^{o}$  were calculated. Thermal decomposition of Au precursor vapor in gas phase was studied by means of in situ high temperature mass spectrometry in vacuum in approximation "isolated molecule". On the basis of presented investigation, the principles of precursor choice were offered for obtaining thin Au films by means of MOCVD, Au layers were obtained. Investigations of thin films were carried out by means of SEM, TEM, AFM and XRD analysis. The influence of precursor nature on structure and morphology of films were demonstrated. The work was supported by Integral Interdisciplinary Project N97 (Siberian Branch of Russian Academy of Sciences) "The fundamentals of processes of chemical deposition of films and structures for nanoelectronics".

O.S.C.II.9.

# MICROSTRUCTURAL DESIGN OF YBCO SINGLE-GRAIN BULK SUPERCONDUCTORS WITH $CeO_2$ ADDITION

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The refinement of Y<sub>2</sub>BaCuO<sub>5</sub> particles is the most useful way to increase critical current density, maximum trapped magnetic field and levitation force of single grain YBCO bulk superconductor. The influence of preparation parameters as nominal composition (Y<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> additions), particle size of starting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> powder, milling and mixing conditions and sintering temperature on the refinement of Y<sub>2</sub>BaCuO<sub>5</sub> particles in the single-grain YBa<sub>2</sub>Cu<sub>2</sub>O<sub>7</sub>/Y<sub>2</sub>BaCuO<sub>5</sub> bulk superconductors prepared by top-seeded melt-growth process has been studied. The microstructure was analysed after sintering and melt processing by polarised light microscopy and electron microscopy. It is shown that cerium is active in the Y<sub>2</sub>BaCuO<sub>5</sub> particle refinement when it is solved in the peritectic melt. When cerium is present as barium cerate, it has not refining effect. The addition of CeO<sub>2</sub> and barium cerate formation even leads to a faster growth of Y<sub>2</sub>BaCuO<sub>5</sub> particles at the sintering stage due to intensive melt production. Refinement of Y<sub>2</sub>BaCuO<sub>5</sub> particles in the samples with large YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> particles is related to the formation of very dense Y<sub>2</sub>BaCuO<sub>5</sub> skeleton which is resistant to melt formation at the sintering stage. Superconducting parameters at the temperature of liquid nitrogen were characterised by magnetisation measurements with vibrating sample magnetometer and by measurement of the profile of trapped magnetic field. Measured critical current density and maximum trapped magnetic field of these single-grain bulk superconductors are significantly influenced by final microstructure, mainly by the size of Y<sub>2</sub>BaCuO<sub>5</sub> particles.

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O.S.C.II.1O.

### ADHESIVE CONTACT OF ROUGH ELASTIC SOLIDS

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New models of normal and sliding adhesive contact between rough elastic bodies with twoterm friction law are presented. Roughness is simulated by the Winkler-Fuss nonlinear elastic layer which can be stretched. Mechanical properties of the layer are determined by statistical theory of adhesive contact between nominally flat rough surfaces. The contact of solids is described by the nonlinear boundary integral equations with non-monotonic operators. Their solutions determine the reduction of effective thickness of rough layer, contact stresses and contact region. For the solving of nonlinear boundary integral equations the method of successive approximations is proposed.

O.S.C.II.11.

# CATALYTIC EFFECTS OF NANO-SIZED TIC TIN Nb<sub>2</sub>O<sub>5</sub> Cr<sub>2</sub>O<sub>3</sub> AND NiCl<sub>2</sub> ON THE HYDROGEN STORAGE PROPERTIES OF LIAIH<sub>4</sub>

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Li alanate recently has emerged as an attractive complex hydride for hydrogen storage and fuel cell application due to its high hydrogen content (10.5 wt%). However, in its pure form the practical utility of Li alanate is limited by slow kinetics, poor reversibility, and high temperatures. Although some catalysts are added to LiAlH4 which has ameliorated not only the kinetics of desorption but also in effect has lowered the effective desorption temperature of LiAlH<sub>4</sub> by eliminating the kinetic restrictions. But the most of these catalysts induce the much reduction in hydrogen storage capacity during the ball-milling. Moreover, it has also been demonstrated to possess a slight reversibility of 0.8 wt.% by doping LiAlH<sub>4</sub> with some catalysts, but to date no conclusive demonstration of reversibility has been reported. Therefore, there have been persistent efforts to explore new effective catalysts that can enhance the reaction kinetics and reversibility while maintaining the high hydrogen capacity. It has been recognized that a refinement of the microstructure (particles and crystallites/grains) of hydrides, most preferably to the nanometric level, accompanied by nanosized catalytic additives may offer several advantages for the physicochemical reactions such as surface interactions, adsorption in addition to bulk absorption, rapid kinetics, low-temperature sorption, hydrogen atom dissociation, and molecular diffusion via the surface catalyst. Therefore it is worth studying the influence of additives in the form of nanoparticles on the hydrogen storage properties of LiAlH<sub>4</sub> [1-2]. In the present work, influence of the catalytic activity of TiC, TiN, Nb<sub>2</sub>O<sub>5</sub>, Cr<sub>2</sub>O<sub>3</sub> and NiCl<sub>2</sub> nanoparticles on the dehydrogenation/rehydrogenation characteristics of LiAlH<sub>4</sub> are investigated by pressure-content-temperature (PCT), X-ray diffraction (XRD), differential scanning calorimatory (DSC), X-ray photoelectron spectroscopy (XPS) and field scanning electron microscopy The doped samples (FESEM). dehydrogenation at much lower temperatures. Doping induced a decrease in the decomposition of first step by about 50°C-65°C compared to that of as received LiAlH<sub>4</sub>. Also, amount of hydrogen release was significantly higher for TiC, Nb<sub>2</sub>O<sub>5</sub> and Cr<sub>2</sub>O<sub>3</sub> additions than that of samples doped with TiN and NiCl<sub>2</sub>. Isothermal desorption results at 120 °C revealed that dehydrating rate of doped alanate was much faster than that of pure LiAlH<sub>4</sub>. TiC, Cr<sub>2</sub>O<sub>3</sub>, Nb<sub>2</sub>O<sub>5</sub>, TiN and NiCl<sub>2</sub> dopants showed the reabsorption of about 1.9 wt%, 1.8 wt%, 1.1 wt%, 1.3wt%, and 1.1 wt%, respectively. XRD, XPS and FESEM analyses suggested that TiC, TiN and Cr<sub>2</sub>O<sub>3</sub> were stable during the ball milling as well as the dehydrogenation processes. On the contrary, NiCl<sub>2</sub> reacted and caused the partial decomposition of Li alanate during the ball milling process, whereas Nb<sub>2</sub>O<sub>5</sub> reduced during the ball milling and rehydrogenation resulting in the low valence state niobium oxide compounds.

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O.S.C.II.12.

# COMPLEX EFFECT OF NANOFILLER ON STRUCTURE AND PROPERTIES OF POLYMER-MODIFIED EPOXY

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Nanofillers of various geometry can lead not only to reinforcement, but also significantly affect phase behavior of multicomponent polymer systems. In melt mixed thermoplastics, they influence the dynamic phase behaviour of immiscible components. Even more complex effect of nanofillers come into account in polymer-modified epoxy in the course of curing reaction induced phase separation of modifier, initially dissolved in liquid resin. In this case influencing of reaction kinetics, nucleation of phase separated domains and miscibility of components by suitably modified nanofiller must be considered. In the case of phase separation by nucleation and growth mechanism, the effect of nanofiller on diffusion and viscosity is especially important.

This work deals with the effect of layered silicate and double hydroxide on structure and behaviour of epoxy/liquid poly(oxyalkylenes) and nitrile rubbers systems with various functionality. The size of phase separated particles and its dependence on clay content was strongly dependent on temperature, which (determines) influences the balance between major nanofiller-effects mentioned above. As a result, both decrease and increase of particle size with clay content in the range 0.5 - 5% in dependence on temperature occurred. The corresponding mechanical properties indicate that suitable nanofiller-polymer combination may lead to favourable balance of mechanical properties, i.e., synergistic combination of clay-induced effects occurs. Best results were found in case of blended organic inorganic structures, consisting of clay tactoids and fine polymeric inclusions obtained by preblending of functionalized polymer with nanofiller. In the case of application of analogous nanofiller-polymer compound (adduct), formation of lamellar self assembled structure was found. Basic aspects determining its formation and structure/properties relationships including fracture mechanics are discussed.

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PL.S.III.1.

# ASSEMBLY OF HIERARCHICALLY SCALED SEMICONDUCTOR NANOSTRUCTURES

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I will discuss how we have combined the short range processes of strain-induced self assembly with longer range lithographic forcing functions to create semiconductor nanostructures arrays that can be controlled over many orders of magnitude of length scales. Our work uses the input of positional maps from focused ion beam pulses that locally modify Si substrate surfaces to template the subsequent assembly of (Si)Ge nanostructure arrays through epitaxial growth. We examine the transfer functions that translate the original template maps into the observed distributions of nanostructures in the assembled array, and show that it is possible to accurately template nanostructure arrays over length scales ranging from nanometers to macroscopic dimensions. I will also discuss novel focused ion beam methods to deliver pulses of electronic or magnetic doping species with doses as small as a few ions per pulse and positional accuracy of order ten nm. With such methods we hope to functionalize ordered nanostructure arrays to develop prototype nanoelectronic devices based on motion of just a few units of electronic charge or spin. Finally, I will discuss how we use a new organizational architecture to integrate the complex multi-variable set of kinetic processes involved in synthesis of these arrays, the "materials cladogram".

Work in collaboration with J. Floro (UVa), J. Gray (U. Pittsburgh), Frances Ross (IBM), M. Gherasimova (S. Connecticut State), A. Portavoce (CNRS), P. Balasubramanian, S. W. Chee and J. Murphy (RPI).

PL.S.III.2.

# INTERFACE AND DEFECT PHENOMENA OF SEMICONDUCTOR OXIDE NANOSTRUCTURES

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Advanced high-resolution imaging and spectroscopic techniques of electron microscopy play a crucial role in characterizing the microstructure and the structure-property relationships of inorganic materials and interfaces. The presentation will describe applications of quantitative transmission electron microscopy methods to investigations of surface and interface phenomena of nanostructured oxide semiconductors grown by a thermal method from powder precursor materials.<sup>1-4</sup> Such material systems are of potential interest for applications in nanoelectronics, spintronics, or solar cells. For ZnO, nanorods form that contain voids, precipitates, and tubular voids with liquid Sn-rich fillings when doped with Sn. Thin surface layers of a spinel phase form by interfacial reactions. The Sn-rich core material is found to reversibly melt and expand under different thermal loads exerted by the microscope electron beam. The growth and the defect formation are related to diffusion processes, similar to the Kirkendall mechanism. Growth inhomogeneities and formation of spinel phases occur for doping with Ga and Al, respectively. Cathodoluminescence spectra show a blue-shifted ZnO band gap luminescence which is often attributed to the effects of doping. For In<sub>2</sub>O<sub>3</sub>, tubular cavities or "nanopipes" of constant diameter form in nanorods along their total length. More complex defect structures, consisting of nanoprecipitates, dislocation loops, and voids, are observed in the core of Sn-doped In<sub>2</sub>O<sub>3</sub> nanorods. These phenomena are related with dislocation-driven growth mechanisms.

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PL.S.III.3.

# EXPLORING THE ARCHITECTURE OF SOLID SOLUTIONS WITH ATOM PROBE MICROSCOPY:

### A PATHWAY TOWARDS REMARKABLE NEW MATERIALS PROPERTIES

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Metallic (not glassy!) aluminium alloys with ~1 GPa yield strength? Magnetic carbon? Microstructure control that enhances both strength, and ductility? How? In this lecture, I will discuss pathways to achieve these technologies through solute engineering in solid solutions — via the creation of particular *solute architectures*.

The challenge for this research frontier is to be able to make actual observations of the solute architecture that can feed back into processing schemes and materials models. Short range ordering, atomic clustering, segregation and site-occupancy are major issues that influence phase transformation pathways and kinetics, and consequently the properties and performance of many technologically important supersaturated solid solutions, including 3rd generation photovoltaic semiconductors, spintronic ceramics and many structural alloys. Scattering based approaches using X-rays, neutrons or electrons to detect and precisely measure this 3D atomic architecture in the solid solution are extremely challenging because of complex convolutions in the diffracted intensity – so much so, that it is unlikely general solutions can be implemented.

I will discuss our approach to addressing these issues using atom probe microscopy. We have recently modelled the origins of resolution in atom probe, and computed advanced spatial distribution maps, which are largely analogous to Patterson functions in scattering experiments. This has enabled us to devise an approach for 'lattice rectification' of the atom probe data, somewhat analogous to aberration correction in TEM. The results are taking us closer to the dream of full 3D atomic resolution microscopy, and are revealing a complex hierarchy and architecture of atomic structures within solid solutions that can be manipulated to influence materials properties – and so contribute to the achievement of remarkable new materials properties.

PL.S.III.4.

### THE FUTURE OF MAGNETIC DATA STORAGE

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Hard-disk drive magnetic data storage began in 1956 with the IBM Random Access Method of Accounting and Control (RAMAC) system that could store 5 Mbytes of data on fifty 24 inch disks with an areal density of 2 kbits/in<sup>2</sup>. Today's commercially available magnetic data storage devices have areal density approaching 500 Gbits/in<sup>2</sup>, an increase of over 200 million times. Although development of more sensitive read-back heads that use a Giant Magnetoresistive (GMR) spin valve device contributed to this Moore's Law like behavior, improvements in the magnetic recording thin-film media are equally responsible. In fact, future increases in the areal density will depend upon solving fundamental limitations of the present media materials. Current commercially available magnetic media use sputtered cobalt alloys with additions of platinum and chromium having an average grain size of ~ 8 nm. In order to continue increasing the areal density requires reducing the magnetic grain size so that noise from the bit transitions does not overwhelm the read-back signal. However, cobalt alloys become thermally unstable, i.e., superparamagnetic, at smaller grain sizes where the magnetization of individual grains will randomly switch from thermal excitation. Therefore, new materials are being considered for future media, such as L1<sub>0</sub> ordered FePt alloys with exceptionally large magnetocrystalline anisotropy  $(K_n)$ . High  $K_n$  materials would allow for thermally stable grains less than 3 nm in size and support areal densities in the Terabit/in<sup>2</sup> regime. Processing FePt media with Terabit/in<sup>2</sup> areal density will require a monodispersed 3 nm grain size, perfect L1<sub>0</sub> order, crystallographic alignment of the tetragonal c-axis, and non-magnetic isolation between the grains. High-resolution transmission electron microscopy (TEM) will play a major role in overcoming the many challenges facing the development of these future magnetic data storage devices.

PL.S.III.5.

# SIZE-DEPENDENT MAGNETIC PROPERTIES OF SINGLE IRON-BASED NANOPARTICLES PROBED BY X-RAY SPECTROMICROSCOPY

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Local control of magnetization dynamics in magnetic nanoparticles is one of the biggest challenges in materials science. To this end, an improved understanding of the spin configuration close to the single- to multi-domain transition is highly relevant. This is difficult in ensemble measurements due to the role of interparticle interactions and also because essential effects of particular morphological parameters, preferential crystallographic orientations upon growth or specific substrate defects may be averaged over. In this work, we combine photoemission electron microscopy (PEEM) with synchrotron x-ray magnetic circular dichroism (XMCD) to study element-specific magnetic properties of single 5-25 nm iron (Fe) metal particles prepared by a gas-phase cluster source [1-2] and 10-30 nm iron oxide (Fe<sub>3-x</sub>O<sub>4</sub>) particles synthesized by high-temperature decomposition of an organic iron precursor [3], deposited on various substrates. For Fe particles in contact with magnetic supports, we find a transition from an exchange-dominated to an anisotropy-dominated regime at a size of 6 nm leading to a spin-spiral structure in the particles above the critical size [1]. For particles supported on non-magnetic substrates, the transition from a blocked ferromagnetic regime to a superparamagnetic phase could be detected by combined temperature- and angular-dependent studies in a range of 120 K to 400 K. The XMCD spectra of the single Fe nanoparticles show that the spectral shape of both the isotropic absorption and the dichroic signal is retained for particles down to 6 nm and is in reasonable agreement with that of metallic bulk Fe [2]. The isotropic spectra of 10 nm and 17 nm Fe<sub>3-x</sub>O<sub>4</sub> nanoparticles cannot be fully superimposed to those of reference magnetic iron oxide species, preliminarily indicating that the surface stoichiometry of the nanoparticles might be different.

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PL.S.III.6.

### MAGNETISM AND MAGNETIC MATERIALS FOR NONVOLATILE MEMORY

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STT-RAM is expected to be the most promising candidate among the next generation memory thanks to the realization of 'spin-transfer-torque(STT)' phenomena and the success in the MgO barrier fabrication. Two major prerequisites for STT-RAM to be commercialized are (1) the reduction of a critical current density for switching a magnetic bit in STT-RAM to the order of 1 MA/cm² and (2) the attainment of magnetoresistance larger than 200% at RA of 10  $\Omega\mu\text{m}^2$  or smaller. A magnetic tunnel junction (MTJ) structure with layers having an out-of-plane anisotropy or with a synthetic free layer has turned out to provide potential solutions for the reduction of the switching current density. We have fabricated MgO-based MTJs with various synthetic free layers and those with layers having out-of-plane anisotropy. A high magnetoresistance and large exchange-bias field can be obtained simultaneously by adopting an in-situ annealing during the deposition of multilayers. The paper will report how their tunnel magenetoresistance (TMR) and critical switching current density (J<sub>c</sub>) are influenced by the structure and materials of multilayers and the fabrication processes.

PL.S.III.7.

### TOROIDAL METAMATERIALS

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We present a new class of artificially engineered electromagnetic materials (so-called metamaterials), the resonant response of which cannot be attributed to the excitation of conventional magnetic or charge multipoles and can only be explained by the existence of the induced toroidal dipole. Toroidal moments are fundamental electromagnetic excitations that cannot be represented in terms of the standard multipole expansion [1]. They were first considered by Zel'dovich back in 1957 [2], but only recently have become the subject of growing interest owing to their peculiar electromagnetic properties. Electromagnetic interactions with toroidal currents were predicted to disobey such widely accepted principle as the actionreaction equality. Toroidal currents can also form charge-current configurations generating vector potential fields in the absence of radiated electromagnetic waves. Although toroidal moments are held responsible for parity violation in nuclear and particle physics, no direct evidence of their importance for classical electrodynamics has been reported so far. This is because effects associated with toroidal moments in naturally available materials are extremely weak and usually masked by much stronger effects due to conventional electric and magnetic dipole and quadrupole moments. Here we demonstrate classical systems, i.e. metamaterials, the electromagnetic response of which is directly related to the resonant excitation of the toroidal dipole moment. The resonant toroidal response has been observed in 'metamaterial slabs', twodimensional arrays of artificially engineered electromagnetic scatterers (metamolecules) of toroidal symmetry. To emphasize the toroidal response we came up with special designs of the metamolecules, where both electric and magnetic dipole moments induced by an incident electromagnetic wave (as well as higher multipoles) are substantially suppressed, while the toroidal response is spectrally isolated and resonantly enhanced to a detectable level. Since toroidal excitation is routinely neglected in the constitutive relations, boundary conditions, electromagnetic forces and in the calculation of momentum loss and radiation intensity of charge-current configurations, we believe that our results indicate a need for the revision of some aspects of electrodynamics involving structures of toroidal symmetry. Furthermore, given that many biologically important molecules have elements of toroidal symmetry and may support toroidal moments such a revision could unveil new mechanism of intra-molecular interactions and genetic information transfer.

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PL.S.IV.1.

### BEHAVIOR OF RADIATION EFFECTS IN NANOMATERIALS

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The nanomaterials are the non-equilibrium objects in general due to the great interface presence (including concentration segregations, residual stresses, etc) and it causes to relate with a special attention to the real exploitation conditions influence on these materials structure and properties. It is obvious that such objects under the thermal action or the stress, corrosion and radiation fields will suffer some processes connected with recrystallization, segregation, homogenization and relaxation, phase transitions, phase decay and arising, amorphization, sintering and filling of micro- and nanopores (nanocapillars). All these processes lead to a nanostructure evolution or even to its annihilation that is accompanied with the changes of its physical, chemical, mechanical and other properties. The questions of the nanostructures stability are of special interest because this problem has not only a theoretical value but have the big applied importance too, for both the nanomaterial stability and their economic effectiveness predictions. The information about the nanomaterials behavior under an irradiation is very important especially for the design and creation the perspective materials for the nuclear units new generation (fast-neutron reactors, high-temperature gaseous reactors, thermonuclear reactors, etc), because their operational conditions presuppose a long-term exploitation in the strong radiation fields under the high temperatures, severe stresses and corrosive surrounds. Now the information on radiation stability of nanomaterials is limited and scattered. This report is an attempt to generalize these data. The much attention is given to some possible results of the nanomaterials irradiation such as the interphase role as the radiation defect sinks, the nanostructure amorphization, the nanocrystallization of amorphous state, the alloying component segregation, and the enhancement of recrystallization. The radiation effects are analyzed in connection with the structure and physical/mechanical properties of nanomaterialsbased metals and alloys (Ni, Cu, Ag, Pd, W, Cu/V, austenitic and ferritic steels, etc.) as well as compounds (TiNi, TiN, ZrO<sub>2</sub>, SiC, etc.). These data include results as applied to realized both by ion irradiation in accelerators and neutrons in reactors. The results of microscopic approaches and the molecular dynamics modeling are also described. Some low investigated questions are pointed and discussed. The important role of nanotechnology in development of new radiation damage-resistant materials is underlined.

PL.S.IV.2.

# SYNTHESIS AND PHOTOCATALYTIC CHARACTERISTICS OF CARBON-TiO<sub>2</sub> HYBRID NANOWIRES AND NANOBELTS

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One-dimensional TiO<sub>2</sub> nanostructures such as nanowires, nanotubes, and nanobelts have been extensively studied for promising applications in the elimination of pollutants, water splitting for hydrogen generation, solar cells, and Li-ion batteries. Recently, much attention has been focused on hybridization of TiO<sub>2</sub> with carbon structures and modification of TiO<sub>2</sub> by carbon doping to exploit the full potential of TiO<sub>2</sub> for such applications. It has been reported that C-TiO<sub>2</sub> hybrid nanostructures enhanced the photocatalytic reactivity because the composites slowed the recombination rate of photogenerated electron-hole pairs. It has also been known that C doping was very effective to extend the photocatalytic reactivity of TiO<sub>2</sub>, whose bandgap energy is ~3.0-3.2 eV, to visible light regime. The formation of 1-D C-TiO<sub>2</sub> hybrid nanostructures is essentially based on a two-step process, either TiO<sub>2</sub> coating on carbon nanostructures such as CNTs or carbon coating on 1-D TiO<sub>2</sub> nanostructures such as TiO<sub>2</sub> nanotubes. In this presentation, we report two one-step synthesis methods for C-TiO<sub>2</sub> hybrid nanowires and nanobelts: (i) metalorganic chemical vapor deposition; (ii) thermal treatment with methanol and ethanol vapors. The methods not only produce high-density C-TiO<sub>2</sub> hybrid nanowires and nanobelts without the use of any metal catalysts such as Au, but also provide self-doped carbon for efficient visible-light photocatalysis. More importantly, TiO<sub>2</sub> nanowires and nanobelts seem to be grown via self-formed nanographitic layer, thus, appear to be a C-TiO<sub>2</sub> hybrid form. We will further discuss the self-catalytic growth mechanism and photocatalytic characteristics of the C-TiO<sub>2</sub> nanowires and nanobelts.

PL.S.IV.3.

# THE REVOLUTIONARY RTILS ROOM TEMPERATURE IONIC LIQUIDS AT ELECTRIFIED INTERFACES: FROM UNDERSTANDING TO APPLICATIONS

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Plasma in a bottle? This is a reality nowadays, with the recent explosion of research in strongly correlation coulomb systems – room temperature ionic liquids (RTILs) – 'the so called 'solvent-free electrolytes'. Practically unlimited number of these non-volatile smart substances can be synthesised in laboratory and mixed to optimize the target applications, ranging from energy generation and storage (batteries, solar cells, fuel cells, and supercapacitors) to electroactuators and lubricants, from extraction of metals to catalysis, from cosmetic industry to gating in molecular electronics. A large class of applications is related with their structure and properties at electrified interfaces, including nano-templated electrodes. This lecture will overview the current status of understanding of the electrical double layer in RTILs near electrodes surfaces as a function of voltage, as well as of various devices based on it. Existing theories and computer simulations will be confronted with reported experimental observations.

The presentation will cover:

- Results for flat electrodes,
- Results for more 'realistic' electrodes, including nano-templated electrodes,
- The link between the structure and dielectric response of the double layer and the properties of nanotemplated supercapacitors, electroactuators, and lubricants.

The talk will discuss not only equilibrium properties, but also some features of the dynamic response of the double layer to charging and discharging, including the ion transport dynamics in confined geometries. Overview-like in character, it is intended to compare different, sometimes contradicting, but often complementary achievements of different groups worldwide. But it will also highlight a set of latest original results, based on joint projects of the presenter's group at Imperial (including those with S. Kondrat) in cooperation with the groups of Maxim Fedorov (Max Planck Institute, Leipzig), Martin Bazant (MIT), Yuri Gogotsi (Drexel University), and few others.

PL.S.IV.4.

# SILVER AND ALUMINUM BASE NANOCOMPOSITES PREPARED FROM BALL MILLED POWDERS

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Mechanical alloying was used to prepare starting components for two types of composites consolidated using powder metallurgical methods. The first one intended for electric contact materials consists of nanocrystalline silver, strengthened with either tungsten, or an amorphous phase additions. The other one designed as a high strength low density material, was prepared using hot pressing of milled nanocrystalline aluminum 7475 alloy with Al<sub>2</sub>O<sub>3</sub> or ZrO<sub>2</sub> ceramic phase additions. Composites were prepared from silver with 20 or 40% W additions, known already as good electric contact materials. They were consolidated from milled powders and showed an increase of hardness with an addition of tungsten, however it was lower (90 HV) than that of the composite with the amorphous phase addition (100 HV) in case of 20% of the amorphous phase addition. Structure studies have shown some refinement of tungsten particles after milling, particularly at their surface, where layers of small particles of tungsten within silver were observed. Small amount of tungsten is incorporated into silver solid solution after milling in spite of the complete lack of solubility of tungsten in silver in the solid and liquid phase. Tungsten precipitates formed after hot pressing causing strain field contrast formation around precipitates. The microstructure of Ag-W composite after hot pressing is essentially similar to that with the addition of the amorphous phase, consisting of fine amorphous particles with nanocrystalline intermetallic inclusions within the nanocrystalline silver matrix. The contact erosion studies performed up to 50000 of cycles indicated similar contact erosion properties of both types of composites indicating a good perspective of silver-amorphous composites for contact materials. The aluminium alloy base composites were prepared from ball milled pre-alloyed 7475 aluminum powders with ceramic particles for 40 hours to obtain grain refinement down to the nano range. The milling was performed in a high energy planetary Fritsch ball mill for 40 hours. TEM studies indicated solid solution grain size refinement after milling down to the range of 30-40 nm. The powders were compacted using uniaxial press in vacuum at 380°C and 600 MPa. The microstructure investigations proved that both types of composites show a uniform dispersion of ceramic phases and no agglomeration was observed, indicating positive effect of milling. The composite matrix was characterized by fine grain size, i.e. less than 100 nm and contained a high density of intermetallic, Zn, Cu or Fe rich phases. The EDX chemical analysis indicated local presence of MgO phase at the metal/Al<sub>2</sub>O<sub>3</sub> interfaces. The microhardness of consolidated samples were in the range of 315-355 HV range for composites with 10-20 % of nano-Al<sub>2</sub>O<sub>3</sub> additions. The compression tests indicated compression strength up to 1000 MPa at a few percent of plastic strain until failure.

PL.S.IV.5.

### MICROBIAL ASPECTS IN CORROSION STUDIES

- FEMS Lecturer Award for Excellence in MSE 2010 -

### J. Michalska

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Microbial structures grow practically everywhere, on all kind of materials, in almost any environment where there is a combination of moisture, nutrients, and a surface. That's the reason why they are present on a variety of surfaces – from stones and plants in aquatic environments to industrial systems, and even human bodies. The most heavily microbial activity is present in industrial equipments. Microbiological deterioration of water quality induces biofouling and biocorrosion. We could observe damages ranging from microelectronic products to reduced efficacy of heat exchangers, unexpected corrosion of stainless steel or premature destruction of mineral materials.

Microbially influenced corrosion (MIC) has been focusing increasing attention from different research areas in the last years, as an answer to the demand of wide variety of industries and degradation cases. The difficulty in reaching an adequate understanding of corrosion processes induced by microorganisms has result in cross-fertilization of ideas between researchers from different disciplines like microbiology, electrochemistry, metallurgy and materials engineering. Different MIC mechanisms can be simultaneously or alternately occurring on various materials, where a complex boundary layer of corrosion products, bacterial cells and other environmental factors are present on the surface. The paper discusses new aspects of MIC mechanisms induced by sulphate reducing bacteria species, taking into consideration modern techniques and new approaches in the study. Practical cases concerning microbial risks, failures illustrate the complexity of these phenomena: from local corrosion problems through stress corrosion cracking. Microbial aspects in hydrogen damage phenomena are discussed. Tensile stresses in SCC, and biological activity in MIC, must be responsible for producing a distribution of embrittlement source, generally hydrogen, with a synergic effect between both phenomena. The role of microstructure and chemical composition of materials is also highlited as a key factor in microbial damaging. In addition to this, the principal morphologies of attack and cracking are described.

PL.S.IV.6.

# AFM-RAMAN-SNOM AND TIP ENHANCED RAMAN STUDIES OF MODERN NANOSTRUCTURES

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We demonstrate instrumental realization and various applications of Atomic Force Microscopy integrated with Confocal Raman/Fluorescence/Rayleigh microscopy and Scanning Near Field Optical Microscopy (SNOM) produced by NT-MDT. Results on various samples are demonstrated: graphene, carbon nanotubes, semiconductor nanowires, quantum dots, nanodiamonds, plasmonic waveguides, photonic crystal optical fibers, various biological objects etc.

For example, graphene on gold is investigated by different AFM and spectroscopy techniques providing comprehensive information about the sample. We study in details how the thickness (number of monolayers) in graphene affects its physical properties: surface potential (work function), local friction, elastic modulus, capacitance, conductivity, charge distribution, Raman and Rayleigh light scattering etc. Results for graphene flakes are qualitatively compared to those for carbon nanotubes of different diameters. We show how electrostatic charging of graphene flakes can be effectively measured and modified by AFM cantilever. Studies are performed both in ambient air conditions and in controlled atmosphere and humidity.

We also present results of Tip Enhanced Raman Spectroscopy (TERS) or "nano-Raman" mapping realized using integrated AFM-Raman system. Measurements are realized in two different excitation configurations: Inverted (for transparent samples) and Upright (reflected light configuration, for opaque samples, with side illumination option). In both geometries we demonstrate near field Raman enhancement effect due to resonant interaction of light with localized surface plasmon at the apex of a metal AFM probe. Various samples are studied by TERS technique: thin metal oxide layers, fullerenes, strained silicon, carbon nanotubes, graphene. Actual plasmonic and near field nature of the Raman enhancement is proven by a number of ways: dependence of the enhancement on the excitation wavelength and polarization, enhancement versus tip-sample distance curves, observation of selective enhancement of Raman signal from thin surface layers of the sample etc. Finally, the ultimate performance of TERS is demonstrated by measuring Raman 2D maps with subwavelength lateral resolution (down to 14 nm) – determined not by the wavelength of light, but by the localization area of the surface plasmon electromagnetic field. We discuss current progress in manufacturing reliable TERS probes.

O.S.E.1.

# MECHANOCHEMICAL SYNTHESIS AND CHARACTERIZATION OF II-VI NANOCRYSTALS: CHALLENGE FOR CYTOTOXICITY ISSUES

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CdSe@ZnS nanocrystals have been prepared by a two-step solid state mechanochemical synthesis. CdSe prepared from elements (milling I) is mixed with ZnS synthesized from zinc acetate and sodium sulphide (milling II). The crystallite size of the new type CdSe@ZnS nanocrystals determined by XRD Rietveld refined method was 35 nm and 10 nm for CdSe and ZnS, respectively. ED/TEM/EDS methods show good crystallinity of the nanoparticles and SEM elemental mapping illustrate consistent distribution of Cd, Se, Zn and S elements in the bulk of samples. UV-VIS spectra show an onset at 320 nm with calculated band gap 3.85 eV. This absorption arises from the vibration modes of Zn-S bonds. The nanocrystals show the blue shift from the band gap of bulk ZnS (3.66 eV). The synthesized CdSe@ZnS nanocrystals have been tested for dissolution, cytotoxicity and *L*-cysteine conjugation. The dissolution of Cd was less than 0.05 µg/ml (which is the detection limit for Cd determination by atomic absorption method). The very low cytotoxic activity for selected cancer cell lines has been evidenced. The synthesized nanocrystals were successfully coated with *L*-cysteine. The obtained organically modified CdSe@ZnS nanocrystals are water-soluble and have a great potential in biomedical engineering as fluorescent labels in cancer treatment.

O.S.E.2.

# MEMBRANE BIOREACTOR BIOFOULING AS EXTRACELLULAR MATRIX: AN INNOVATIVE STRATEGY FOR MATERIALS DESIGN

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The extensive use of membrane bioreactors (MBR) has been delayed by membrane biofouling (B). MBR-B is often described as an extracellular matrix in which biopolymers (BP), inorganics and microbes co-exist. Ultrafiltration (UF) trials using organic scaffolds (chitosan and albumin) and colloids (CaCO<sub>3</sub>) were conducted in order to mimic MBR-B sequence. Either constant pressure UF or step-pressure trials were assessed. MBR-B properties (hydraulic resistance –R-, permeability –K-, organic to inorganic matter ratio –o/i-, compressibility –n-, specific membrane mass) were determined. Pore-blocking was estimated via mathematical models. Colloid addition to BP resulted in K decreases and R increases. BP-CaCO<sub>3</sub> UF produced compressible skins on polymeric membranes (n = 0.6-1.2; thickness = 0.6-2  $\mu$ m, o/i = 1-2). A roadmap for MBR-B development was set forth based on biomineralization arguments and it will be utilized as root to explain the way by means MBR-B mimicking acts as driving force for advanced biomaterial design and it depiction via fractal dimension.

O.S.E.3.

# MULTIFUNCTIONAL NANO PARTICULATE SYSTEMS BASED ON HYDROXYAPATITE AS SYSTEMS FOR LOCAL DELIVERY OF VITAMIN D3

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Multifunctional drug delivery system based on hydroxyapatite may be a research challenge in the treatment and reconstruction of bone tissue. Vitamin D3 has a positive effect on osteogenesis as it increases osteoblast differentiation and mineralization of bone tissue.

The purpose of the study presented in this paper has been to examine the possibility of the synthesis of a new multifunctional nanoparticulate system for local delivery of vitamin D3 suitable for applications in bone engineering. The synthesis, characterization and application of three nano particle systems was shown: hydroxyapatite, hydroxyapatite/vitamin D3 and hydroxyapatite/PLGA/vitamin D3.

The obtained vitamin D3-loaded nanoparticles based on hydroxyapatite. Characterization was performed with wide-angle X-ray structural analysis (XRD), infrared spectroscopy (FT-IR), field-emission scanning electron microscopy (FESEM), zeta potential (ZP) and particle sized distribution (PSD) methods. Basic *in vitro* studies were performed implantation of materials in rats. XRD and FT-IR analyses confirmed that the vitamin D3 is loaded hydroxyapatite and PLGA. Different values of zeta potential may refer to different phenomenological processes during *in vivo* studies.

O.S.E.4.

### ANTIBACTERIAL ACTIVITY AND CYTOTOXICITY OF HYDROXYAPATITE/SILVER NANOCOMPOSITES SYNTHESIZED BY A SONOCHEMICAL APPROACH

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Hydroxyapatite, as a major constituent of the inorganic part of natural human bones, is a natural choice and one of the most frequently applied materials for the reparation and regeneration of bone tissue. The formation of composites based on HAp, the incorporation of foreign ions within its structure and/or the functionalization of their surfaces allow improvements to the morphological, structural and surface properties. Such improvements can be utilized to increase the material quality for applications in dentistry and orthopedics as well to extend the potential applicability in other fields of biomedicine.

Hydroxyapatite/silver (HAp/Ag) nanocomposite particles were formed using the sonochemical method. Particles were formed from HAp rods with silver (present in the form of ions) incorporated within the apatite structure and/or metallic particles, embedded into apatite rods and metallic particles attached to the surfaces of these rods. The so obtained materials were tested for antibacterial activity. The p presence of the bacterial growth-inhibition zone around the discs made of composite material and the fluorescence dye detection on the surface of the HAp/Ag composite (corresponding to the labeled live and dead bacteria) proved that the composite was active against both Gram-positive and Gram-negative bacteria. In addition, it was determined that the minimal inhibition concentration (MIC), i.e., the minimal concentration of HAp/Ag composite, which is able to inhibit the growth of bacteria, was higher for Grampositive (MIC = 0.7-0.8 mg/ml) when compared to Gram-negative (MIC = 0.6-0.7 mg/ml) bacteria. The same effect was determined during the investigation of the minimal bactericidal concentration (MBC) of the HAp/Ag composite against the same representatives of Grampositive and Gram-negative bacteria. The obtained concentrations of the HAp/Ag composite which were able to manifest the bactericidal effect were used for an investigation of the toxicity against the representatives of healthy and cancer-modified cell lines. The toxicity of a composite was investigated in vitro and for that purpose the IMR-90 human lung embryonic fibroblast and U-2 OS human osteosarcoma cell lines were applied.

In the presentation the antibacterial activity of the HAp/Ag composite and its toxicity against human cells will be discussed.

O.S.E.5.

# NONINVASIVE OPTICAL SENSING OF GLUCOSE IN WATER SOLUTION, BLOOD, AND HUMAN TISSUES

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About 140 million people worldwide suffer from diabetes mellitus, and manage it on a daily basis by measuring their glucose level. This often requires frequent lancing and finger bleeding. Glucose, a monosaccharide, is a very important substance for human metabolism. There are two optical isomers of glucose, D- and L-glucose. However, only D-glucose is involved in human metabolism. As opposed to current, quite invasive tests for glucose detection, a noninvasive method offers numerous advantages. These include the absence of pain, lack of biohazard materials, and the potential for better disease management, among others.

In this vein, we performed experiments to determine glucose levels in an aqueous solution, whole blood, and tissues (blood vessels in the skin and eyes) in order to examine glucose concentration. However, *in vivo* noninvasive blood glucose sensing is very challenging due to very weak glucose signals. To overcome these difficulties we developed a novel, noninvasive optical method that can detect glucose concentration from 4-20 mmol/L, with a resolution of 0.1 mmol and having 84.96 % accuracy, and compared it with the lancing method, a golden standard (Accu-Chek Active, Roshe Diagnostics GmbH). Our research results are based on the first initial group of 63 respondents (16 healthy people and 47 people with diabetes). Research is in progress, and we plan to increase accuracy and to apply this method for sensing glucose in both the skin and eyes blood vessels.

O.S.E.6.

### FORCE MEASUREMENTS ON TEETH

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Fixed dental braces are designed to correct the false alignment of teeth. They are composed of brackets that are attached to the tooth and the wire is usually made from shape memory alloy NiTi. Wires are constructed to link the teeth so that they always act with a force. General characteristics of optimal orthodontic force those are light and continuous. Based on clinical research are optimal forces and torques to move the teeth depend on the type of teeth and tooth direction and they are usually between 0.1-2 N and 1-50 Nmm. Insufficient forces and torques are ineffective and may extend the duration of treatment. Conversely, excessive forces and torques can lead to severe pain, or parodontal damage and root resorption. For these reasons, it is necessary to know what forces are caused by each individual wire.

The main advantage of NiTi orthodontic wires compared to conventional ones is their ability to deliver constant stress to push the teeth into the proper position. This property makes this product much more efficient, thus reducing the length of orthodontic treatment for patients.

In the last few years research in this area has focused on accurate measurement of the forces and torques on the teeth in all three directions as a result of the actions of orthodontic wires. For these purposes some "real" experiments were also made to determine these forces and torques.

In this paper we present different techniques of force measurements and our preliminary results of case study with finite element method, which was made using the Abaqus computer programme. With this numerical method we will try to define the forces caused by different types of super-elastic NiTi wires, which are attached to the labial surface of teeth at various angles, on teeth. In doing so, we will establish what stress the wires cause on the periodontal ligament. With regard to the permissible stress in the periodontal ligament we will define the characteristics of super-elastic wire. On the basis of the results and properties we will give guidance and a directive for selecting the optimal wire.

Key words: force measurments, NiTi orthodontic wires, Abaqus programme.

O.S.E.7.

# TECHNOLOGY OF PRODUCTION OF ANTIOXIDANTS PREPARATIONS FROM PLANT MATERIALS

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Antioxidants play one of the main roles in protection of normal vital functions of organisms. Increasing of antioxidant status of organism can be provided by the consumption of additive quantities of antioxidant. The main sources of antioxidant are plant extracts. Current technologies of production of extracts are based on liquid processes. Because of antioxidants are reducers, they have strongly activity with oxygen and intermediates of oxidizing of organic compounds. Decreasing of yield of antioxidants, nonreproductivity of concentrations, problems with storage are technical effect of high activity of antioxidants. It is known that stability of reducers in the solid phase in comparison with those in the liquid phase is strongly higher. We showed availability of using of solid phase mechanochemical reactions for producing of preparations of unstable antioxidant compounds from plant material. The ratio of oxidizing of active component – hypericin from St. John's Wort and catechins from Green tea in the solid mechanochemical preparation in comparison with those in liquid preparation was decreased not less than 500 times. The yield of active components increased in 2-10 times.

O.S.E.8.

# DESIGNING MOLDS FOR RAPID ROTATIONAL FOAM MOLDING OF INTEGRAL-SKIN CELLULAR POLYOLEFIN COMPOSITES

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Rapid Rotational Foam Molding is a novel patent-pending technology developed for efficiently processing fine-celled integral-skin cellular polyolefin composites by exploiting the synergistic effects resulting from the deliberate conjunction of extrusion with rotational molding. Thereby, a distinct fine-celled foamed layer or core within the interior of hollow moldings can be encapsulated entirely within a solid skin integrated boundary layer while reducing the processing cycle time and the energy consumption to a fraction of previously common levels. However, for implementing successfully the rapid rotational molding process the rotational molds had to be specially designed. This paper introduces the specific functional requirements the mold design had to satisfy through presenting several iterations of the design parameters such as the mold interface, the mold venting, and the mold shape. Three typical mold shapes: a cylindrical, a flat plate and a box mold have been subjected to a comparative experimental study to validate the design solutions through the obtained product quality.

# Poster Presentation

P.S.A.1.

# NANOCOMPOSITES OBTAINED BY HIGH PRESSURE TORSION POWDER CONSOLIDATION

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Heavy plastic deformation at relatively low homologous temperatures is usually called severe plastic deformation (SPD). Different SPD methods exist where High Pressure Torsion (HPT) is one of the preferred techniques due to several advantages. The aim of the paper is to present a special powder compaction technique with the HPT method. This new approach permits with the generation of composites or even nanocomposites by SPD where similar microstructures as during mechanical alloying can be generated. Nevertheless, one advantage of the HPT powder consolidation method is given by the complete abstinence of a sintering treatment. Bulk samples of different types of nanocomposites are obtained directly during SPD processing. It will be shown that arbitrary material combinations can be selected.

P.S.A.2.

### THE ISOELECTRIC POINT OF ZIRCONIA

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The isoelectric point,  $pH_{iep}$ , of laboratory prepared zirconia sol in KNO<sub>3</sub> and  $K_2SO_4$  solutions of various concentrations was investigated at  $25^0$  C. Zirconia sol was prepared from zirconyl oxychloride solutions by forced hydrolysis at  $102^0$  C. The prepared sol was monodispersed (with Polydispersity index, PdI, equal to 0.074) and consisted of almost spherical, monoclinic, hydrated zirconia particles 65 nm in diameter. The isoelectric point was determined by a potentiometric method using a Zetasizer Nano instrument equipped with a MPT-2 Autotitrator (Malvern, UK). The influence of the electrolyte concentration (0.001 -0.1 M KNO<sub>3</sub> and  $10^{-5} - 10^{-3}$  M  $K_2SO_4$ ) on  $pH_{iep}$  was investigated. The obtained  $pH_{iep}$  of zirconia in KNO<sub>3</sub> solutions was  $7.5 \pm 0.1$ , while those in  $K_2SO_4$  solutions (from  $10^{-5}$  to  $10^{-5}$  M) were from 7.3 to 5.0, respectively. The decrease in  $pH_{iep}$  values with an increase in  $K_2SO_4$  concentration indicates specific sorption of sulfate ions on the zirconia surface. Simultaneously, the particle size of zirconia was measured. As shown, the particle size of zirconia increases with increasing dispersion pH due to agglomeration of zirconia particles, reaching the maximum value at  $pH_{iep}$ .

P.S.A.3.

# HYDROTHERMAL SYNTHESIS OF ZIRCONIUM SUBSTITUTED HYDROXYAPATITE

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Aim of work is to investigate an efficiency of hydrothermal treatment on formation of zirconium substituted hydroxyapatite  $Ca_{5-x}Zr_x(PO_4)_3OH$ . A set of trial was conducted to optimize process and find substitution limit. Molar ratio of Zr/(Ca+Zr) in precursor suspension was varied from 0 to 0.2 with step of 0.05. Powders were analyzed by means of techniques such as XRD, Fourier transform IR spectroscopy, ICP, laser - diffraction granulometry and SEM.

P.S.A.4.

### COLD PLASMA TREATMENT OF POLYMERIC MATRIX COMPOSITES

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Atmospheric pressure plasma is a fast, clean surface treatment. It does not generate any environmental waste, and it is highly effective to improve adhesion properties through surface energy increase. This work studies the effect of plasma treatment on a glass fibre reinforced epoxy used in construction applications, as well as in the plain epoxy matrix.

Two plasma torch speeds were selected: 1 and 10 m/min. Contact angle measurements were carried out with water, glycerol and diiodomethane, both immediately after surface treatment and after 30 days. Data were analyzed using Owens-Wendt-Rabel-Kaelble (OWRK) method to calculate surface energies. A big effect on the polar part of the energy was found. A pull-off test is used to evaluate changes on adhesion.

Keywords: Composites, plasma treatment, surface energy, contact angle.

P.S.A.5.

# MECHANICAL MILLING PROCESS OF A PETROLEUM COKE WITH BORIC ACID FOR LITHIUM-ION BATTERIES

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The effect of mechanical grinding on doped carbon precursors (boron doped petroleum coke) has been studied. The material was subjected to planetary milling and attritor milling at two different speeds (400 and 700 rpm) for different times (1, 5, 10 and 15 h). The doped material was characterized by SEM, XRD, TEM and XPS. The results show that it is possible to introduce foreign atoms such boron into the carbon lattice intentionally by the milling process, which is the meaning of doping. Boron is one of the few elements which are known, with some certainty, to enter substitutionally into the carbon lattice. The petroleum coke has shown high activity through the milling process, absorbing a great quantity of oxygen. As a result, the potential of boron-substituted carbons in the lithium-ion batteries is increased relatively to unsubstituted carbon.

Keywords: Petroleum coke; Milling process; boron doping, lithium-ion batteries.

P.S.A.6.

# EFFECT OF PLASMA MODIFICATION ON SURFACE PROPERTIES AND CHEMICAL STRUCTURE OF CHITOSAN/GELATIN/PLLA FILMS

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Films casted from organic solution of chitosan/gelatin/PLLA blend (52/13/35 wt-%) were treated by dc discharge (working gas - air, 50 mA, 60 sec). The blend was obtained by Solid-State Reactive Blending in a twin-screw extruder at 100°C. The films treated at the cathode or anode possessed enhanced hydrophilicity in comparison with untreated one ( $\theta_{water}$ =36, 40 and 71°, respectively). According to XPS data, plasma treatment resulted in the decrease of oxygencontaining groups and the appearance of nitrogen-containing ones. Study of the surface topography showed that the untreated film possessed homogenous structure, whereas plasma treatment led to local destruction which was more pronounced at the anode treated film. The ability of the prepared films to support attachment and growth of animal cells was tested using L-929 cell line (mouse fibroblasts).

P.S.A.7.

### THE POSSIBILTIES OF THE MECHANOCHEMICAL MODIFICATION OF MoO3

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It was found that mechanochemical modification of  $MoO_3$  (orthorhombic modification) in different media leads to the change of its crystalline structure: i) the fast formation of monoclinic modification of  $MoO_3$  at dry treatment, ii) existence of orthorombic and monoclinic modifications mixture at treatment in ethanol, iii) formation of sidvilite phase  $MoO_3 \cdot nH_2O$  after treatment in water. The prepared samples were studied using XRD, XPS, SEM, ESR, AFM and XANES methods. It was found that while the initial  $MoO_3$  has low activity and selectivity in ethanol oxidation, the sample after treatment in dry atmosphere shows very high activity and selectivity to acetaldehyde. The presence of sidvilite phase leads to formation of the catalysts with high selectivity to ethylene. Applying the mixture of monoclinic and orthorhombic phases as a catalyst enables the simultaneous formation of ethylene and acetaldehyde.

P.S.A.8.

### RHEOLOGICAL PROPERTIES OF BIOPOLYMER MEMBRANS AND FRICTION EFFECTS

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The complex phenomenon of transport inside and through the biopolymer membranes is related to many biomedical applications, targeted release of active substances at nano-level and understanding some basic living processes. For example nano-engineering process of hemoglobin intra-cellular transport control through erythrocyte and out of it under hypotonic condition can be used for different further applications. It includes conductive and convective mechanisms.

In this contribution we consider experimentally and theoretically changes of membrane conditions during sealing time period. The driving forces of convective transport are considered in particular radial lipid membrane fluctuations as the result of the decrease of the erythrocyte volume. In this way is obtained profiles of hemoglobin concentration that represents the results of convective and conductive mechanics. The Langevin-type equation is developed for modeling the radial fluctuations dependently on the rheological characteristics of lipid membrane formulated at mesoscopic scale.

P.S.A.9.

# LOCAL DENSITY EFFECTS OF POLYMER NANO-STRUCTURED FILLER COMPOSITES

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One of most pronounced effects of polymer composites with active fillers is its ability to dramatically change strength of the material. The effect is known more than hundred years but the reinforcing mechanism is still poorly understood. It is believed that the primary reinforcing mechanism has its origin in some peculiar features of particle-polymer interactions. Very high filler surface area is necessary for reinforcement but it is not enough for making differences between various filler types and even grades of the same filler.

One possible explanation are differences in nano –structure of surface layer of different filler grades. Using integral equations for pair correlations we consider in this contribution effects of nano- structure for different fillers. Such differences in particle morphology change local density of polymer around the filler particles as our experimental and numerical results indicate.

P.S.A.10.

# MICROSTRUCTURE AND PROPERTIES OF LaCoO<sub>3</sub> PEROVSKITE THIN FILMS DEPOSITED BY LASER ABLATION PROCESS

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LaCoO<sub>3</sub> perovskite thin films have been deposited by pulsed laser deposition technique on the surface of Si and MgO single crystal substrates. Samples have been prepared with different values of the laser pump energy, 30J and 35J. The results affected for the change of energy were generally the thin film thickness, the quantity and the size of droplets over the thin film surface. The microstructure, chemical/phase composition and morphology of prepared thin films were examined by means of diverse techniques (SEM, TEM, EDS, XRD and XPS). For the surface topography observations of thin films the Atomic Force Microscopy (AFM) was applied. Nanohardness and scratch tests (adhesion measurements) were also performed for estimation of perovskite films mechanical properties and quality. Obtained results confirm that PLD technique allow to carry stoichiometric composition of functional compound from the target to the single crystal substrate however the microstructure and properties of obtained thin films are highly influenced by the laser ablation parameters (laser wavelength, energy density, time and target-substrate distance).

Keywords: microstructure, LaCoO<sub>3</sub> perovskite, pulsed laser deposition.

P.S.A.11.

# SYNTHESIS AND CHARACTERIZATION OF LiM<sub>x</sub>Mn<sub>2-x</sub>O<sub>4</sub> CATHODE MATERIAL USING STARCH COMBUSTION METHOD

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The spinel type  $LiMn_2O_4$  is usually used as cathodic material for rechargeable lithium-ion batteries owing to its advantages such as low cost, non-toxicity and thermal stability. It is known that the substitution of a part of Mn ions by the ions of other transition metals such as Cr, Co and Ni, may improve the electrochemical properties of  $LiMn_2O_4$ . In this study, original  $LiMn_2O_4$  spinel and its substituted analogue  $LiCr_{0.15}Mn_{1.85}O_4$  were synthesized by a starch combustion method. The spinel structure of the obtained powders was confirmed by X-ray diffraction. The SEM microphotographs indicated uniform spherical particles of average size of about 200 nm. Electrochemical performances were studied by cyclic voltammetry in aqueous electrolyte.  $LiCr_{0.15}Mn_{1.85}O_4$  shows some lower discharge capacity than  $LiMn_2O_4$  (92 versus 110 mA h g<sup>-1</sup>) but process intercalation/ deintercalation  $Li^+$  for the substituted spinel was more close to a reversible one.

P.S.A.12.

### SURFACE CHARACTERISTICS OF CARBONIZED HEMP ACTIVATED WITH POTASSIUM HYDROXIDE

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Possibility of producing activated carbon material from waste short hemp fibers is described. Five samples were obtained using different temperature of carbonization and various amounts of potassium hydroxide as activated agent. Adsorption and desorption isotherms of  $N_2$  were measured on all activated samples, at -196°C. The specific surface area, pore size distribution, mesopore including external surface area, and micropore volume were calculated. Nature and thermal stability of the surface oxygen groups were investigated by temperature programmed desorption method. Adsorption properties of obtained samples were tested by adsorption of pesticides (acetamiprid, dimethoate, nicosulfuron, carbofuran and atrazine). The samples carbonized at higher temperature exhibit increase in specific surface area ( $S_{\rm BET}$  up to 2192 m²/g) and amount of surface oxygen groups. Also, specific surface area and the amount of surface oxygen groups depend on the amount of KOH. All tested samples were microporous and activation with higher amount of hydroxide slightly increases the mesoporosity. Obtained results showed that all samples have good adsorption properties, and decrease pesticides initial concentration of 500 ppb for more than 90 %.

P.S.A.13.

# CHARACTERISTICS OF THE THERMAL OXIDATION OF THIN POLYSILICON FILMS GROWN BY LPCVD AND HEAVILY IN SITU BORON-DOPED

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In this work, we present a comparative study between first and second thermal oxidation properties of low pressure chemical vapor deposition (LPCVD) thin polysilicon films. These films are heavily in situ boron-doped with a concentration level of around  $2x10^{20} cm^{-3}$ . Their properties are analysed using electrical and structural characterization means by four points probe resistivity measurements and X-ray diffraction spectra. The thermal-oxidation processes are performed on sub-micron layers of  $200 nm/c\mathchar`-Si$  and  $200 nm/SiO_2$  deposited at temperatures  $T_d$  ranged between  $520\mathchar`-C$  and  $605\mathchar`-C$  and thermally-oxidized in dry oxygen ambient at  $945\mathchar`-C$ . The study made shows by comparison, the oxidation of in situ doped films typical a very large increases of both the surface oxidation rate  $K_s$  and oxide diffusion coefficient D even when the film deposition temperature  $T_d$  decreases. Compared to the as-grown resistivity with  $T_d$  is known to be in the following sequence  $<\rho_{520}><<\rho_{605}>$ . The measure X-ray spectra is shown, that the Bragg peaks are marked according to the crystal orientation.

Keywords: Oxidation, Si-LPCVD, In situ doped boron, Deposit temperature.

P.S.A.14.

### INFLUENCE OF ATTRITION MILLING ON BARIUM TITANATE PROPERTIES

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Barium titanate (BT) as the ferroelectric material is a good candidate for variety of applications due to its excellent dielectric, ferroelectric and piezoelectric properties. In this work barium titanate powder was prepared by soft chemical process from polymeric precursors (modified Pechini process). The obtained BT powder was nanosized with primary particles ~ 74 nm, but factor of agglomeration (Fagg) pointed on presence of agglomerates ~ 6 µm. It is well known that agglomerates could influence on setback of materials structure and properties. In order to obtain the de-agglomeration of nanopowder and to improve BT properties, an attrition milling was performed. Barium titanate powder was treated in attrition mill with zirconia media for 1h in 2% polyacrylic acid. Milled powder (BTA) possessed particles ~ 50 nm and agglomerates size was reduced to ~ 690 nm. Specific surface area of milled powder was higher than in starting BT powder. To investigate the effect of milling on electrical properties of ceramics, both BT powders were uniaxially pressed and sintered at 1300 °C for 8 h in air. SEM micrographs showed polygonal grains with dimensions around 2 µm in both ceramics. On the other hand, density of ceramics obtained from milled powder was 95 % of theoretical value and 90 % for BT. Temperature dependence of relative permittivity showed three structural transitions characteristic for ferroelectric BT ceramics. The temperature transition from ferroelectric to paraelectric was found to be at 120 °C for BT and 122 °C for BTA. Dielectric constant value was around 6700 for BTA, which was much higher value in comparison with non-treated BT where permittivity was 1340. Dielectric losses were below 0.03 in both BT ceramics.

P.S.A.15.

# MECHANOCHEMICAL ACTIVATION OF THE REACTION BETWEEN SILICA AND CATECHOL

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The soluble monomeric forms of silicon are biologically active. However, silicon dioxide, the most widespread silicon compound, is highly soluble only in alkaline medium. The mechanochemical reaction of amorphous silicon dioxide with catechol has been used for solubilizing silicon dioxide at neutral pH. By studying the kinetics of solubilizing the silicon dioxide - catechol system, the mechanism of the reaction between polyphenols with silicon dioxide has been suggested. This mechanism involves the interaction of hydroxyl groups on the silica surface with catechol, the formation of surface complexes and transferring them into solution. Relying on this mechanism, the method for targeted modifying the surface has been suggested. This method allows increasing the efficiency of the process and the solubulization rate.

### P.S.A.16.

# MAGNETORESISTANCE EFFECTS IN FERROMAGNETIC CHALCOPYRITE SEMICONDUCTORS

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The nano-sized magnetic clusters are the source of an above room temperature ferromagnetism observed in several Mn doped chalcopyrite II-IV-V<sub>2</sub> compounds. The presence of magnetic clusters significantly modifies electrical properties of  $Zn_{1-x}Mn_xGeAs_2$  and  $Cd_{1-x}Mn_xGeAs_2$  crystals. In this contribution, the results of the magnetoresistance studies in the high magnetic fields and at low temperatures will be presented. The  $Zn_{1-x}Mn_xGeAs_2$  crystals showed giant magnetoresistance effect with maximum amplitudes around 50% due to the charge carrier tunneling and the spin polarization in nano-size ferromagnetic grains. In the case of  $Cd_{1-x}Mn_xGeAs_2$  samples with the composition x=0.028, the effect is substantially higher, and the large linear positive magnetoresistance, with maximum values of about 550% (B=22 T) for is observed. The results are interpreted in terms of the geometrical magnetoresistance model.

P.S.A.17.

### PREPARATION AND CHARACTERIZATION OF NANO FERRITES

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The nanosized NiFe<sub>2</sub>O<sub>4</sub> and MnFe<sub>2</sub>O<sub>4</sub> powders were prepared by mechanochemical synthesis in a Fritsch planetary ball mill during various milling times (3 h to 25 h). The natures of these powders were confirmed by various techniques, such as XRD, SEM, TEM, IR and Raman spectroscopy. Magnetic measurements and Mössbauer spectral studies indicated that the as-prepared NiFe<sub>2</sub>O<sub>4</sub> and MnFe<sub>2</sub>O<sub>4</sub> ferrites are typical for soft ferromagnetic materials. This simple, cost-effective, and environmentally friendly method that produces no by-product effluents can be used to synthesize pure crystalline spinel nickel and manganese ferrite nanoparticles. Furthermore, it can be extended to synthesizing other spinel ferrite nanoparticles of interest in nanotechnology.

P.S.A.18.

# THE INFLUENCE OF THE DETONATION SPRAYING PARAMETERS ON THE PHASE COMPOSITION AND MICROSTRUCTURE OF TiO<sub>2</sub>-Ag COATINGS

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In the present work,  $TiO_2$  (rutile) - 2.5 vol.% Ag composite powers were sprayed using a detonation gun with acetylene as a fuel. We showed that flexible control over the spraying parameters - the composition of the explosive mixture ( $C_2H_2+O_2$ ) and its volume - opens up possibilities of tailoring the phase composition, microstructure and surface morphology of titanium oxide-based coatings. Reduction of  $TiO_2$  to  $Ti_3O_5$  occurred in the coatings deposited under a reducing atmosphere when particles reached a molten or a semi-molten state. With larger volumes of the explosive mixture filling the detonation gun, higher temperatures and velocities of the particles could be achieved. Increasing oxygen content in the explosive mixture led to much higher temperatures of the sprayed particles. In the coatings sprayed using a stoichiometric  $O_2/C_2H_2=2.5$  mixture, the major phase was rutile.

P.S.A.19.

### SYNTHESIS AND STRUCTURE OF COPPER(II) COMPLEX WITH PYRIDOXALAMINOGUANIDINE AND O-PHENANTROLINE

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Study of coordination chemistry of pyridoxalaminoguanidine (PLAG), started by Leovac et al., resulted in a limited number of the complexes characterized so far. However, since both ligand-precursors and the ligand itself have been known for significant biological activity, it seems worth of continuing examination of possibilities of synthesis of other metal complexes with PLAG. Here we present synthesis and structure of square-pyramidal Cu(II) complex with PLAG and o-phenantroline (phen). PLAG is coordinated in zwitter-ionic form, in a usual tridentate ONN mode, *via* atom of phenolic hydroxyl and nitrogen atoms of azomethine and guanido group. Slightly deformed square-pyramidal environment of Cu(II) is achieved by the coordination of chelate ligand and one N atom of phen in equatorial plane and the other N atom of phen in the apical position.

P.S.A.20.

### STRUCTURE AND PROPERTIES ZIRCONIA AND THEIR EVOLUTION AFTER LOW TEMPERATURE ANNEALING

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It has been studied the influence of low temperature annealing of  $ZrO_2$ - $Y_2O_3$  powder on its structure and properties. It has been shown, that the increasing of temperature led to the decreasing of an average particle size and the increasing specific surface for low temperature and finally to the increasing grain size and the decreasing specific surface. It has been determinated the activation energy and grain growth is defined by surface diffusion.

P.S.A.21.

### THERMOGRAPHIC PROPERTIES OF EUROPIUM DOPED YTTRIUM-GADOLINIUM OXIDE NANOPHOSPHOR

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Phosphors are thermographic if they exhibit emission-changing characteristics with temperature. In this sense phosphor thermometry represents temperature measurement technique that utilizes changes of photoluminescence properties of phosphor with temperature. Temperature affects phosphors emission in several ways giving the phosphors temperature sensing characteristics. The changes of electron transition intensities are strongly affected by temperature and the intensity ratio between two emission lines in is widely accepted as a temperature sensor since the intensity ratio measurements eliminates a number of errors from fluctuations of the excitation light source, temperature changes of excitation bands and non-uniform dopants' concentrations.

Knowing that yttrium and gadolinium oxides have high chemical stability and temperature resistance, we investigated possibility for their usage in phosphor thermometry by observing temperature changes of trivalent europium transitions from  $^5D_1$  and  $^5D_0$  energy levels, introduced into yttrium-gadolinium oxide nanostructured matrix  $((Y_{0.75}Gd_{0.25})_2O_3:Eu^{3+})$  as dopant. Measurements were recorded in from room temperature up to 820 K, showing that  $(Y_{0.75}Gd_{0.25})_2O_3:Eu^{3+}$  nanophosphor is a new promising high temperature thermometric phosphor with very good sensitivity.

P.S.A.22.

# INFLUENCE OF MECHANICAL ACTIVATION ON THE ELECTRICAL AND MAGNETIC PROPERTIES OF FERRITE POWDERS

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Commercial manganese zinc ferrite powder was activated in a planetary mill for 1 hour, 2 hours, 4 hours, 6 hours, 8 hours and 12 hours. Thermo magnetic measurements in non-isothermal conditions at temperatures from room temperature to 600°C showed that the optimal activation time is 6 hours.

It was shown that during the first heating magnetization of the sample milled for 6 hours rapidly decreases with the Curie temperature of 280°C. The cooled sample has got about 16% higher magnetization than the initial magnetization before the heating. In the second warm-up magnetization is increased in the whole temperature range with the Curie temperature of 340°C. After the second heating up to 420 °C magnetization of the cooled sample is about 20% less than the initial magnetization of the sample before the first heating. Thermoelectric measurements in the temperature range from the room temperature to 600°C have proved that the results of these measurements are in complete correlation with the thermo magnetic measurements.

P.S.A.23.

## LINEAR AND NONLINEAR OPTICAL SPECTRA FOR INTERSUBBAND TRANSITIONS OF CORE/SHELL (CdSe/ZnS BASED) SPHERICAL QUANTUM DOTS

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Quantum dots (QD) investigated in this paper are of core/shell/shell structure. In simple case CdSe core is surrounded by ZnS, and in more complicated case by ZnS and CdSe shells, respectively. The electronic structure and optical properties of one-electron quantum dot were investigated by assuming a spherically symmetric confining potential of finite depth. The energy eigenvalues and wave functions dependence on QD radius and structure were calculated by using effective mass approximation. We have calculated energies of s, p and d states, oscillator strengths and the linear and third-order nonlinear intersubband optical absorption coefficients and refractive-index as a function of the QD structure and dimension for the 1s-1p, 1p-1d and 1p-2s transitions.

Keywords: Quantum dot, Nonlinear optics.

P.S.A.24.

# EFFECT OF ELECTRIC FIELD ON GROUND AND EXCITED STATES D<sup>0</sup> BINDING ENERGY IN CdTe/ZnTe SPHERICAL QUANTUM DOT

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The effect of external electric field on the  $D^0$  ground and excited state energies in a spherical quantum dot was studied. The impurity energy and binding energy were calculated using the analitical method within the effective mass approximation and finite barrier potential. Based on computed energies and wave functions Stark shift energy is examined. The results show that the binding energy of hydrogenic impurity depends on the dot radius and the external electric field strength.

P.S.A.25.

#### LAYERED CORE-SHELL MODEL FOR DELIVERING NANOBIOMATERIALS

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In this paper we will analyze application of nanomaterials in biomedicine, that is to say we will present the recent accomplishments in basic and clinical nanomedicine. Numerous novel nanomedicine-related applications are under development or are in the research phase, and the process of converting basic research in nanomedicine into commercially viable products will be long and difficult. Achieving full potential of nanomedicine may be years of even decades away, however, potential advances in drug delivery, diagnosis, and development of nanotechnology-related drugs start to change the landscape of medicine. Implants, especially in dentistry, due to new biomaterials and thin coatings with specific tasks, but are now widely used. Based on our research in ultrathin crystalline structures performed so far, superlattices, quantum wires and Q-dots, we will consider the core-shell multilayer materials that can act as carriers for medicines and tagged substances.

P.S.A.26.

### ELECTROCHEMICAL PROPERTIES OF ANODICALLY GROWN TiO2

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Nanostructured amorphous and anatase  $TiO_2$  are both considered as high rate Li-insertion/extraction electrode materials. Here we present the preparation of titania on titanium substrate by the anodic oxidation method. The anodization was conducted using a two-electrode configuration under a constant voltage. Highly viscous fluoride containing glycerol electrolyte was used to anodically grow amorphous  $TiO_2$  on titanium substrate. The crystal structure was characterized by X-ray diffraction. After thermal treatment at 400 °C amorphous  $TiO_2$  crystallizes to anatase phase. The surface morphology was observed by scanning electron microscopy. Electrochemical properties of the as-prepared substrates directly used as anode in lithium-ion cell were examined through galvanostatic discharge/charge tests.

P.S.A.27.

# INFLUENCE OF SIC NANOPARTICLES ON THE MECHANICAL PROPERTIES OF $Si_3N_4$ -SIC COMPOSITES

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Silicon nitride and silicon carbide are the promising materials for high temperature application due to their excellent high temperature properties. One of the ways how to improve mechanical properties is the incorporation of SiC particles into silicon nitride matrix. The in-situ reaction of carbon with  $SiO_2$  is a cheap and simple way to produce the  $Si_3N_4$ -SiC micronanocomposite. High temperature properties - creep behaviour, thermal shock resistance, oxidation resistance and tribology of carbon derived  $Si_3N_4$ -SiC micro-nanocomposite and monolithic  $Si_3N_4$  has been studied. The presence of SiC particles refined the microstructure of  $Si_3N_4$  grains and caused the change of mechanical properties. Present work try to explain basic phenomena influenced the resultant mechanical properties and shows the positive but also negative influences of SiC particles on some of the high temperature mechanical properties.

P.S.A.28.

### THE INFLUENCE OF A FORCED FLOW ON DENDRITIC GROWTH IN BINARY MELTS

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The effects of a forced flow on dendritic growth rate in binary systems are studied theoretically. By using the Oseen approximation of the Navier-Stokes equation, the linear stability analysis and the solvability criterion, one determines a scaling factor as a function of the velocity of the forced flow and the impurity concentration in the melt in the three-dimensional model. The criterion obtained rallies analytic results for dendrite growth under forced convection in a pure system and dendrite growth in a stagnant binary system.

P.S.A.29.

### RECENT ACHIEVEMENTS IN INVESTIGATIONS OF BAYER ALUMINUM TRIHYDROXIDE GROWTH

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Despite the fact that Bayer process is discovered long time ago, there are still unknowns especially in the field of aluminum trihydroxide growth. It has long been known that gibbsite crystallize in a monoclinic system but its morphology is pseudohexagonal as a result of twinning. Aluminum trihydroxide crystals occur in a large variety of shapes and sizes depending of supersaturation: plate-like lozenges, plate-like hexagons and prisms. The basic morphology is lozenge-shaped crystals, while the plate like hexagons and prisms are results of single or multiple twinning, dislocations and presence of impurities. The dominant faces are basal (001) and the prismatic (100) and (110) faces. These faces grow via different growth mechanism. Birth and spread is the most probable growth mechanism of basal faces while prismatic faces grow by spiral growth mechanism at a lower supersaturation. This statement is derived from kinetic analysis of aluminum trihydroxide growth. But, using the SEM and AFM, only confirmed growth mechanism is birth and spread mechanism.

Different growth equations for growth of aluminum trihydroxide crystals from caustic soda solutions have been proposed, but generally square power is considered for the growth rate dependence on the supersaturation in all cases. This may imply that growth of aluminum trihydroxide crystals occur in a spiral fashion what is not consistent with results of microscopy investigations. But, it is also founded that the value of growth order can be different from 2 depending on the supersaturation. So from this point of view the spiral growth model couldn't be an appropriate model to describe the aluminum trihydroxide crystals growth and proposed square power dependence growth rate on the supersaturation is questionable and therefore should be further analyzed.

P.S.A.30.

### CHEMICAL PRECIPITATION SYNTHESIS AND CHARACTERIZATION OF Zr-DOPED HYDROXYAPATITE NANOPOWDERS

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The great importance of hydroxyapatite in the field of biomaterial science inspires researchers to investigate various approaches to adjust and improve existing and to find out new useful properties of this class of materials. Doping of original hexagonal apatite crystal structure with a number of ions has been shown to improve phase stability, mechanical and electrical properties, as well as its biological applicability. Fabrication of Zr-HAp materials could be significant for mechanical properties improvement, teeth implant color adjustment, altogether with conserved bioactivity and without cell toxicity.

In this study, simple chemical precipitation is used to synthesize zirconium-doped hydroxyapatite, Zr-HAp, with 0, 1.0, 5.0 and 10.0 at.% of Zr. Phase purity was investigated by XRD, particles morphology by electron microscopy, while middle range arrangement and presence of different functional groups through IR and Raman spectroscopy studies. Efficiency of Zr-ions incorporation is checked by EDX chemical analysis.

P.S.A.31.

#### CASTABILITY OF ALUMINIUM ALLOYS

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Castability is the ability of an alloy to be cast without formation of defects such as cracks, segregations, pores or misruns. Alloy dependent phenomena that determine castability are fluidity, macrosegregation, hot tearing and porosity. These phenomena have been known for a long time but have only recently become well understood and work is underway to develop predictive castability models. These models require input of physical properties, such as solidification path, dendrite coherency, solidification shrinkage and interdendritic permeability. Some of these properties are difficult to determine experimentally but new experimental techniques are being developed to extract such data. This paper will review the phenomena that limit castability of aluminium alloys. The influence of alloy composition on fluidity, macrosegregation, hot tearing and porosity will be described. Models for castability prediction will be briefly reviewed and data on coherency, fluidity, permeability and shrinkage will be presented.

P.S.A.32.

### ELABORATION OF POROUS INSULATING MATERIALS STARTING FROM ALGERIAN FIRECLAYS

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This study describes a new technique of fabrication of a porous refractory materials starting from fireclay which comes from a deposit located in "Djebel Debbagh" region, in the Algerian east. This material is composed mainly by kaolinite and halloysite, fusible compound such iron and alkalis are less than 1 %. The amount in alumina (in dry state) exceeds 38 % whereas the tenor of silica is lower than 42 % what indicates the absence of free silica. DD3 is very suitable to manufacture of refractory materials, such high-temperature fire bricks. We employed a method which is similar to that which is used to manufacture the clays foam; interconnected materials are obtained at dry state starting from barbotine of clays and foaming agents. The density of this porous refractory material does not exceed 1000 kg/m<sup>3</sup> which showed that porosity is more than 60 %. The compressive resistance is appreciable, and the temperature of melting is > 1650 °C. The expansion as a function of temperature is regular on a large interval of temperature from 25 to 1200 ° C, and the coefficient of thermal expansion is lower than 5x10<sup>-6</sup> °C<sup>-1</sup>. The structure in form of foam confers high heat insulation to this porous refractory material, and can be used to manufacture bricks for the wall of the medium in the construction of furnaces and they act as thermal insulation, insuring heat retention. Often furnace build is realized by 3 or 4 walls of refractory bricks. The bricks which are en contact with fire are dense and must resist the corrosive attack and ensure the stability of the wall, whereas the bricks of the medium ensure the conservation of heat.

Keywords: Elaboration, porous material, fireclay, insulating.

P.S.A.33.

### THE COMPARATIVE PROPERTIES OF SINTERED PRODUCTS BASED ON CLAYS FROM THE MINE BAUXITE "BIJELE POLJANE"

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The deposits of white bauxite "Bijele Poljane" is characterized by the presence of clays with different mineral composition. In this paper it was investigated comparative characteristics based on two types of white clays from the mine bauxite "Bijele Poljane". Comparisons were made in terms of volume shrinkage, total porosity and compressive strength. The samples was formed by plastic shaping in a mould corresponding to a parallelepiped with dimensions of 7.7 cm x 3.9 cm x 1.6 cm. Previously the characterization of examined type of clays was done (determination of chemical and mineral compositions, density, humidity and determination of grain size distribution). The linear and volume shrinkage were determined during drying in air and in a dryer to constant mass at temperature of 110 °C. The samples were sintered at the temperatures of 800 °C, 900 °C, 1100 °C and 1200 °C. For the sintered products there were determined linear and volume shrinkage during sintering, total porosity and compression strength as well as mineral composition of sintered products (X-ray analysis) and microstructure of sintered products (microscopic analysis). On the basis of obtained results there were compared the properties of sintered products in terms of volume shrinkage, total porosity and compression strength in dependence of mineral composition of the investigated type of clays.

P.S.A.34.

### PREPARATION AND CHARACTERIZATION OF Pt NANOCATALYST ON TUNGSTEN BASED SUPPORT FOR ALKALINE FUEL CELLS APPLICATIONS

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Platinum nanocatalyst on tungsten based support has been synthesized and characterized as catalyst for oxygen reduction reaction in  $0.1~\text{mol}~\text{dm}^{-3}$  NaOH solution. Tungsten based support -WxC has been synthesized by modified Ganesan et al. procedure. Synthesized support was characterized by BET, XRD and cyclic voltammetry techniques. Specific surface area of the support determined from nitrogen adsorption/desorption isothermal curves was found to be  $177~\text{m}^2~\text{g}^{-1}$ .

Platinum nanocatalyst at WxC support has been synthesized by borohydride reduction method and characterized by XRD and TEM techniques. It was found homogenous Pt nanoparticles distribution over the support, without pronounced particle agglomeration. Electrochemically active surface area of the catalyst determined from adsorption/desorption charge of hydrogen atoms, after double layer charge substraction, taking into account the reference value of 210  $\mu$ C cm<sup>-2</sup> for full coverage with adsorbed hydrogen species, was found to be 40 m<sup>2</sup> g<sup>-1</sup>.

The oxygen reduction reaction at WxC/Pt catalyst has been studied by cyclic voltammetry and linear sweep voltammetry at rotating disc electrode. Single Tafel slope was observed (value of -0.105 mV dec<sup>-1</sup>), close to the slope at high current densities, for oxygen reduction at pure polycrystalline Pt, as well as at Pt nanoparticles. The specific activities, expressed in terms of kinetic current densities per real surface area at the constant potential, of this new catalyst and Vulcan supported Pt were compared. WxC/Pt catalyst exhibited better catalytic activity for oxygen reduction reaction, as well as better durability comparing with Vulcan/Pt one.

P.S.A.35.

## A STUDY ON THE HYDROGEN STORAGE CAPACITY OF Pd - PLATED POROUS ACTIVATED CARBON

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The middle part of a lime (Tilia platyphyllos) tree was heated in the absence of oxygen and subsequently mechanically ground to obtain activated carbon powder. The particle size of the powder ranged from 100 µm to 200 µm. A chemical process was used to deposit palladium nanocrystals of 8 nm to 15 nm in size on the powder. A total of 0.00005 g Pd per 1 g activated carbon (AC-0.005% Pd) was deposited. The DSC method showed good hydrogen absorption by the AC-0.005% Pd powder within the temperature range of 30°C to 280°C. The enthalpy of the first hydration was 28.4 kJ g<sup>-1</sup>. Structural changes during the first hydration induced an increase in enthalpy during the second hydration to 62.4 kJ g<sup>-1</sup>. As a result of the effect of hydrogen spillover from Pd nanocrystals, the hydrogen absorption rate and the hydrogen amount absorbed were considerably higher in the AC-0.005% Pd powder than in the palladium-free activated carbon. The hydrogen absorption mechanism was determined using the temporal dependence of the change in hydrogen pressure within a constant-volume chamber at a temperature of 150°C. Hydrogen absorption was shown to occur by a complex mechanism. During initial hydrogen absorption at 0 s to 200 s, slow dissociation of adsorbed hydrogen molecules on Pd atoms was the rate-determining step. During the second period of time (200-700 s), the slowest stage was the diffusion of H-atoms in C-0.005% Pd powder nanopores.

P.S.A.36.

# THE EFFECT OF STRUCTURAL CHANGES DURING HEATING OF THE Ni<sub>79</sub>Co<sub>18,6</sub>Cu<sub>2,3</sub> AMORPHOUS POWDER ON ELECTRICAL AND MAGNETIC PROPERTIES

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An amorphous powder of Ni<sub>79,1</sub>Co<sub>18,6</sub>Cu<sub>2,3</sub> alloy was electrodeposited from an ammonium solution of nickel, cobalt and copper sulfates on a titanium cathode. Heating resulted in structural changes within the powder that caused considerable changes in its electrical resistivity and magnetic permeability. Differential scanning calorimetry (DSC) showed that structural relaxation and crystallization occurred within the temperature range of 50°C to 350°C and 580°C 650°C, respectively. Structural relaxation caused an increase in relative magnetic permeability. At room temperature, the relaxed sample showed 15% higher magnetization as compared to the freshly prepared sample. Specific electrical resistivity slowly increased with increasing temperature within the structural relaxation temperature range. Within the crystallization temperature range of 580°C to 650°C, there was a sudden decline in electrical resistivity due to an increase in both the electron mean free path and electron state density at the Fermi level. The electrical resistivity of the crystal sample at room temperature was found to be about two orders of magnitude lower than that of the freshly prepared amorphous powder. The electrical resistivity of the sample after crystallization showed a linear increase with increasing temperature. The amorphous nickel/cobalt alloy containing a low amount of copper of about 2.3 wt.% was found to have considerably higher thermal stability than the copper-free nickel/cobalt alloy due to its crystallization at about 70°C higher temperature. The low copper content also induced thermal stability of magnetic domains; hence the higher Curie temperature in this alloy than in the copper-free alloy.

P.S.A.37.

# MONITORING OF HYDROGEN ABSORPTION/DESORPTION INTO PRESSED $Ni_{97,1}Co_{18,6}Cu_{2,3}$ POWDER USING RESISTOMETRY

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The kinetics of hydrogen absorption/desorption in a Ni<sub>97,1</sub>Co<sub>18,6</sub>Cu<sub>2,3</sub> amorphous powder was determined by measurement of its electrical resistivity. The powder was obtained by electrodeposition from an ammonium solution of nickel, cobalt and copper sulfates. The sample was prepared by powder pressing at 100 mPa at a temperature of 25°C. The equivalent diameter of powder particles ranged from 8 to 250 nm. Hydrogen absorption induced an increase in electrical resistivity. The hydrogen atoms adsorbed on the alloy surface penetrate the crystal lattice and transfer their electron to the conduction zone forming H<sup>+</sup> ions, thus causing a decrease in electrical resistivity. The change in electrical resistivity underlies the absorption mechanism proposed. During initial absorption, the slow dissociation of adsorbed H<sub>2</sub> molecules into adsorbed H atoms was found to be the rate-determining step. During the second period of time, the diffusion of H<sup>+</sup> ions in the crystal lattice of the Ni<sub>97,1</sub>Co<sub>18,6</sub>Cu<sub>2,3</sub> alloy was the slowest step. The hydrogen desorption rate in an argon atmosphere is limited by H<sub>2ad</sub> formation; recombination of adsorbed hydrogen atoms, Had, or by the diffusion of H ions from the crystal lattice over a prolonged period of time. The results experimentally obtained were used to determine constant rates and apparent activation energies for both the dissociation of adsorbed molecular hydrogen and the diffusion of H<sup>+</sup> ions in the crystal lattice of the Ni<sub>97,1</sub>Co<sub>18.6</sub>Cu<sub>2.3</sub> alloy.

P.S.A.38.

# PROPERTIES OF THE ELECTROCHEMICALLY OBTAINED $Ni_{65}Fe_{24}W_{11}$ ALLOY POWDER

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A nanostructured Ni<sub>65</sub>Fe<sub>24</sub>W<sub>11</sub> powder was obtained by electrodeposition from ammonium citrate electrolyte within the current density range of 450 to 1000 mA cm<sup>-2</sup>. The chemical composition of the powder was found not to depend upon current density due to the diffusion control of the process of codeposition of nickel, iron and tungsten within this current density range. XRD analysis shows that the powder contains an amorphous matrix having embedded nanocrystals of the FCC solid solution of iron and tungsten in nickel, with an average crystal grain size of 3.4 nm, a high internal microstrain value and a high density of chaotically distributed dislocations. Codeposition current density and electrolyte temperature of 50°C to 70°C do not have a significant effect on the phase structure of the Ni<sub>65</sub>Fe<sub>24</sub>W<sub>11</sub> powder. SEM micrographs show that the electrodeposition of the Ni<sub>65</sub>Fe<sub>24</sub>W<sub>11</sub> alloy results in the formation of two particle shapes: large cauliflower-like particles and small dendritic particles. The cauliflower-like particles contain deep cavities at hydrogen evolution sites. Cavity density increases with increasing deposition current density. Powder particle size depends upon electrolyte temperature and codeposition current density. Smaller powder particles are formed at higher temperatures and at higher current densities. The magnetic properties of the alloy do not undergo changes up to 50°C. Within the temperature range of 50°C to 350°C, during initial heating, relative magnetic permeability decreases reaching the Curie temperature at about 350°C. Upon initial heating up to 400°C, relative magnetic permeability exhibits a 12% increase due to the relaxation process. During relaxation, different domain groups having different thermal stability are created. Following the second heating to 500°C, the magnetic permeability of the alloy cooled to room temperature is about 5% lower than that of the fresh alloy. This is the result of both the crystallization of the amorphous phase of the powder and the crystal grain growth in the FCC phase.

P.S.A.39.

# KINETICS OF CRYSTALLIZATION AND PHASE TRANSFORMATION OF $Fe_{75}Ni_2Si_8B_{13}C_2$ AMORHOUS ALLOY

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The kinetics of structural transformations of the  $Fe_{75}Ni_2Si_8B_{13}C_2$  amorphous alloy under non-isothermal conditions was studied. It was shown that the amorphous alloy was stable up to 723 K, when multi-step structural transformations start, involving formation of stable  $\alpha$ -Fe(Si) and  $Fe_2B$  crystalline phases, and a metastable  $Fe_3B$  phase, their growth and the decomposition of the metastable phase into the two stable phases. A second transformation was observed around 970K, involving recrystallization and conversion of  $\alpha$ -Fe(Si) to  $Fe_2B$ . The kinetic parameters corresponding to each of the steps of the observed structural transformations were evaluated.

P.S.A.40.

### SYNTHESIS OF THE NANOSTRUCTURED YAP:Ce VIA SPRAY PYROLYSIS BY POLYMERIC PRECURSOR SOLUTION

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The yttrium aluminum system  $(Y_2O_3\text{-}Al_2O_3)$  includes three compounds: yttrium aluminum garnet  $(Y_3Al_5O_{12}, YAG)$ , yttrium aluminum perovskite  $(YAlO_3, YAP)$  and yttrium aluminum monoclinic  $(Y_4Al_2O_9, YAM)$ . YAP doped with Ce is well known optical material used as a fast scintillator for synchrotron X-ray experiments. Synthesizing single YAP phase is difficult even through wet chemical processing because of the possible allocations of other phases. Here, we synthesized fine powders of  $YAlO_3$ : $Ce^{3+}$  *via* spray pyrolysis of polymeric precursor obtained by dissolving the corresponding nitrates in ethylenediaminetetraacetic acid (EDTA) and ethylene glycol (EG) solution. Aerosol droplets are decomposed at 550 °C in argon atmosphere. In order to get a pure YAP:Ce phase as-prepared particles were additionally thermally treated in the range from 900 °C to 1100 °C for 12 hours in the air atmosphere. Energy dispersive analysis (EDS) confirmed high particle purity and desirable Y:Al ratio. Also, scanning electron microscopy (SEM) showed changing morphology with increasing the heating temperature. Inner particle structure is analysed by transmission electron microscopy (TEM) while phase identification is performed by X-ray powder diffraction (XRD). Detailed structural analysis is performed through Rietveld refinement in Topas Academic software.

P.S.A.41.

### FORMATION OF SOLIDS FROM THE GAS MIXTURES OF CARBON, NITROGEN AND HYDROGEN AT HIGH TEMPERATURES

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The first synthesis of "covalent solid carbon nitride" [1] was achieved in 1993 by pulse laser ablation of graphite targets combined with an intense nitrogen source. Since then, a various methods have been employed to obtain solid carbon nitride. Some of syntheses are performed *via* chemical vapour deposition (CVD) method, plasma enhanced chemical vapour deposition (PECVD), laser assisted chemical vapour deposition (LCVD).

In the vapour, used in synthesis of carbon nitride *via* these methods, different species (atoms, molecules, radicals, ions, electrons) are formed, among of them the initial molecules for cluster formation, as a connection between the individual (isolated) molecules and the solid state structure.

In this paper we consider the formation of carbon nitride solids as well as of the carbon solids, at high temperatures, from the gas mixtures containing nitrogen and carbon as well as from the mixtures of nitrogen, carbon with hydrogen, since the precursor molecules sometimes used in synthesis, contained hydrogen ( $C_3N_4H_4$ ) too. This process is investigated theoretically by computing the equilibrium compositions of the mentioned gas mixtures. The calculation is performed for temperature range between 500 and 6000 K, for different C/N and C/N/H ratios and for the total pressure in the system of 1 and 5 bars. The mole fractions of 45 species (CN,  $CN_2$ ,  $C_2N$ ,  $C_2N_2$ , C,  $C_2$ ,  $C_3$ ,  $N_2$ , N, etc.) that could be formed under investigated conditions, were determined. From the calculated compositions of the investigated gas systems the conclusions are made concerning the importance of the specific carbon and nitrogen containing molecular species in the formation of solid carbon nitride and solid carbon. Also, the temperature zones with saturated and/or oversaturated vapor of carbon containing species (C,  $C_2$ ,  $C_3$ ...) as well of the carbon and nitrogen containing species as (CN,  $CN_2$ ,  $C_2N$ ,  $C_2N_2$ ...) were determined and the formation of solid carbon nitride *via* different reaction routes was analysed.

[1] Chunming Niu, Yuan Z. Lu, Charles M. Lieber, . Science, 261 (1993) 334.

P.S.A.42.

### FORMATION OF $\gamma$ -AITI INTERMETALLIC INDUCED BY LASER IRRADIATION OF AI/TI NANO-STRUCTURES

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Titanium-aluminides, special  $\gamma$ -AlTi, are promising materials for high temperature wear protection in mechanical applications. Different number of (Al/Ti) bilayers, using a d.c. sputtering method, was deposited on silicon substrates. The samples were irradiated in air by a defocused picoseconds Nd:YAG laser beam with different number of pulses. Compositional and structure analysis were done by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Rutherford backscattering spectrometry (RBS), atomic force microscopy (AFM) and high resolution transmission electron microscopy (HRTEM).

Results show that laser irradiation of multilayered Al/Ti structures lead to formation of AlTi intermetallic phase. Due to formation of aluminum oxide on the surface, the rest of deposited structure is protected from oxidation. In the case of eight or ten (Al/Ti) bilayers some number of layers close to substrate remains unmixed after the laser irradiation. For grater numbers of laser pulses on the sample surface is formed periodic structure (ripples) like a surface waves that covers large area. Period of ripples were 1.4  $\mu$ m and amplitude 100 nm for eight (Al/Ti) bilayers and 200 successive pulses. Evidently, this method represents powerful technique for fast fabrication of  $\gamma$ -AlTi, while the existence of unmixed layers provides good adhesion of formed intermetallic phase.

P.S.A.43.

### SYNTHESIS AND CHARACTERIZATION OF Co(II,) Ni(II) AND Cu(II) COMPLEXES WITH 1-HYDRAZINOPHTHALAZINE BASED LIGAND

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1-Hydrazinophthalazine (hydralazine) has been used over 50 years as an arterial vasodilatator. Despite of this long period, the coordination ability of hydralazines to transition metals is poorly investigated. Accordingly, our aim was to synthesize a new polydentate hydralazine-type ligand and to test its reactivity toward transition metal ions. With carbonyl compounds 1-hydrazinophthalazine reacts readily giving Schiff bases. Its reaction with 2,6diacetylpyridine results in bis(phthalazine-1-hydrazone)-2,6-diacetyl-pyridine dihydrochloride. The new ligand with Co(II,) Ni(II) or Cu(II) acetate forms dark brown crystalline compounds. The crystal and molecular structure of the complexes was determined by single crystal X-ray diffraction. It was found that the ligand is coordinated to the central atoms in its monodeprotonated form, in a tetradentate NNNN fashion. Cobalt(III) and nickel(II) crystallizes with one methanol molecule. In the neutral octahedral Co(III) complex the hydralazine ligand occupies the equatorial plane while the chlorido ligands are in the axial positions. The ligand with Ni(II) gives complex cation of a square planar geometry. The electroneutrality of the complex is completed with a chloride contraion. In the reaction with Cu(II) a square pyramidal neutral complex is formed with a chlorido ligand in the apical position. This compound does not contain enclathrated solvent molecules. The complexes were characterized also by IR spectrometry, conductometric measurements and thermal analysis.

P.S.A.44.

### CHANGES IN THE ELECTRONIC STRUCTURE DURING THE HYDROGEN-INDUCED LITHIUM AMIDE/IMIDE TRANSFORMATION

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The reversible transformation of lithium amide (LiNH<sub>2</sub>) into lithium imide (Li<sub>2</sub>NH) during the absorption/desorption of hydrogen (H) is a potentially important process for H storage applications. However, its investigation is difficult due to the competition of many complicated Li<sub>2</sub>NH structures with ground state energies very close to one another. In order to establish the most probable pathways of the transformation, we have examined the changes in electronic structure of all the relevant molecular species and clusters involved in the processes, using abinitio calculations based either on the linear combination of atomic orbitals (LCAO), or a realspace Green's function formalism. The influence of the replacement of Li with some other elements of interest on the system behaviour has been also investigated in this sense. The cluster calculations were conducted so to link the results obtained for molecules and the density functional theory (DFT) calculations of various crystal structures appearing as the end-points of the process. In this way, an atomic-level insight into the changes of the electronic structure during the H-induced LiNH<sub>2</sub>/Li<sub>2</sub>NH transformation has been obtained. Calculations have revealed that the changes of particular molecular and cluster structures have a determining role during the transformation, and that the appearance of several Li<sub>2</sub>NH structures is the long-range ordering response to particular local ordering possibilities during the process.

P.S.A.45.

# STRUCTURAL CHARACTERIZATION OF MECHANICALLY ACTIVATED MgO-TiO<sub>2</sub> SYSTEM

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Mixtures of MgO-TiO<sub>2</sub> powders were mechanically activated in a planetary ball mill for time interval from 0 to 120 minutes. On thus obtained powders, structural investigations have been performed. N<sub>2</sub> adsorption method was used to determine the BET specific surface area and pore size distribution. Unusual results are obtained: specific surface area continuosly decreases up to 40 minutes of activation and after that increases, reaching its minimun value of 4.4 m<sup>2</sup>/g. The influence of mechanical activation on lattice vibrational spectra was examined by Raman spectroscopy at room temperatures. The differential thermal analysis has been performed in order to investigate thermal behavior of the mixtures, indicating at several endothermal peaks in range of RT to 1100°C. SEM gave information about changes in microstructures, showing the clear decrease in particle size.

P.S.A.46.

### EFFECT OF TEMPERATURE AND pH ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF COBALT FERRITE (CoFe<sub>2</sub>O<sub>4</sub>) NANOPARTICLES OBTAINED VIA THE HYDROTHERMAL METHOD

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In recent years spinel ferrite nanoparticles have been investigated because of their special magnetic and electrical properties. One such magnetic material with an inverse spinel structure is cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>). It has a moderate saturation magnetization, a large magnetic anisotropy, a significant chemical stability and a mechanical hardness. With these properties it can be used in various potential applications, such as recording media, magnetic refrigeration, ferrofluids and drug delivery.

In this work, an effort was made to examine the influence of the synthesis temperature and pH on the structural and magnetic properties of CoFe<sub>2</sub>O<sub>4</sub> nanoparticles that were prepared via the hydrothermal route. X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM) were used to determine the particle size and crystal structure of the assynthesized CoFe<sub>2</sub>O<sub>4</sub> nanoparticles. The results revealed the formation of crystalline CoFe<sub>2</sub>O<sub>4</sub> nanoparticles with a size that depended on both the pH and temperature variations during the process of synthesis. The magnetic properties of the CoFe<sub>2</sub>O<sub>4</sub> nanoparticles were measured at room temperature using a vibrating-sample magnetometer (VSM) which allowed us to measure the saturation magnetization and coercivity. The obtained values were lower than in the case of bulk material (about 80 emu g<sup>-1</sup> and 5400 Oe, respectively) which, we believe, can be attributed to the formation of nanoparticles and can be correlated to the influence of pH and temperature on their formation.

P.S.A.47.

#### KINETICS OF DRUG RELEASE FROM HYDROXYAPATITE

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Release kinetics of various antibiotics from calcium hydroxyapatite (CHA), as one of the most used ceramic materials in bone tissue engineering, was investigated in this study. Antibiotics, in solid state, were mixed with CHA powder and the obtained mixture was compressed into tablets. The release of antibiotics from these tablets was measured in a pH 7.4 phosphate-buffered saline solution at 37 °C by UV-VIS spectrophotometer. A new drug release mechanism, that determines the relationship between pore sizes and drug release rate, is suggested here. It quantifies the drug release kinetics based on pore sizes and pore size distribution.

P.S.A.48.

### REMELTING OF M-CrAIY AIR PLASMA SPRAYED COATINGS BY MEANS OF ALUMINIUM COLD ROLLING AND CONVENTIONAL HEAT TREATMENT

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Air plasma spray technique was used to produce NiCrAlY and CoNiCrAlY coatings on the Inconel 713LC substrate. A certain amount of imperfectly melted powder particles, voids and oxides was also present in plasma sprayed coating microstructure. The aluminium sheet of 99,999 purity was cladded by means of cold rolling onto the coating surface. After the cladding of aluminium was the samples annealed at the temperatures of 650, 660 and 700 °C for different dwell time in argon atmosphere. It was found that the temperature significantly affects the annealing time of resulting coatings remelting. Both M-CrAlY coatings are enriched by aluminium, which enable to create the NiAl and Ni<sub>3</sub>Al phases within the original plasma sprayed coating region. Annealing time also affects remelting of the Inconel 713LC substrate surface. The microstructure of coatings was recorded by scanning electron microscope. Coating thickness and amount of voids were measured by means of image analysis. The concentration of phases was estimated by energy dispersive microanalysis.

P.S.A.49.

# FORMATION OF HYPEREUTECTIC ALUMINIUM ALLOY FROM SACRIFICIAL NICKEL COATING INVESTIGATED BY DIFFERENTIAL THERMAL AND MICROSTRUCTURAL ANALYSIS

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Nickel coating was sprayed from the 99.7 wt.% nickel powder by high velocity oxyfuel technique onto the 99.5 wt.% aluminium sheet surface. After the spraying was the samples annealed up to the temperature of 700, 800 and 1000 °C. The heating rate of the samples of 5 °C / min and cooling rate of 20 °C / min was set up. Formation of binary hypereutectic aluminium alloy was investigated by using differential thermal analysis, metallography and scanning electron microscopy. The 99.5 wt.% and 99.999 wt.% aluminium was also investigated to compare the results obtained. The microstructure of Al-Ni hypereutectic alloy is of aluminium matrix and Al $_3$ Ni eutectic. To estimate the chemical composition of phases the energy dispersive microanalysis was used. With increasing temperature the eutectic coarsen and the particles of primary Al $_3$ Ni phase is started to be formed. The image analysis was applied to measure the resulting undissolved nickel coating thickness and Al $_3$ Ni eutectic parameters.

P.S.A.50.

### PREPARATION OF PLATINUM ELECTROCATALYST BY HYDROGEN ION-BEAM IRRADIATION

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We report a particular method of Pt/glassy carbon (GC) surface formation, based on a 15 keV  $H^{*+-}$  ion beam irradiation of thin  $H_2PtCl_6\times nH_2O$  layer placed over the GC surface. The electrochemical activity of such obtained Pt/GC surface toward oxygen reduction and methanol oxidation was compared with the activity of the Pt deposits obtained by other more common reduction procedures. It was observed that ion beam prepared deposits were well adhered to the GC support, unlike to any other Pt-deposition method. Furthermore, the morphology of both GC support and Pt catalyst as well as the electrochemical activity of Pt catalyst was found to be sensitive to the sign of charge of hydrogen ions. The electrochemical activity of Pt/GC surface obtained by  $H^-$  ion irradiation was higher compared to the Pt deposits obtained by other more common reduction procedures. Taking into account that radiation chemical synthesis in a solid medium is minor to that in a homogeneous liquid medium it appears that irradiation with  $H^-$  ion beam can be a method for obtaining the system with enhanced properties whose applicability could be extended to multi-metallic systems.

P.S.A.51.

# RELATIONS BETWEEN J., M. AND N. INTEGRALS AND THOSE WITH INTERACTIONS ENERGY IN A BRITTLE MATERIAL

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In this study, kinematics of the Damage Zone (DZ) or the so-called Fracture Process Zone (FPZ) which often precedes the crack during its propagation and characterized by few degrees of freedom (elementary movements) such as translation, rotation, isotropic expansion and distortion are considered. On the basis of a stress field distribution obtained by the use of a Semi-Empirical Approach (SEA), which relies on the Green's functions, these driving forces corresponding to the mentioned degrees of freedom are formulated within the framework of the plane problem of elastostatics. Thus, expressions for translation (J), isotrope expansion (M), distorsion (N) and interactions effects representing the active parts of crack driving forces known as energy release rates are formulated in a purely theoretical context.

Keywords: Potential energy, energy release rate, Green's function, process zone.

P.S.A.52.

### SYNTHESIS OF PENTLANDITES WITH VARIABLE COMPOSITION AND PHASE TRANSFORMATIONS UPON HEATING IN INERT ATMOSPHERE AND AIR

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Samples of pentlandites with variable composition (Fe<sub>4.5</sub>Ni<sub>4.5</sub>S<sub>8</sub>, Fe<sub>3</sub>Ni<sub>6</sub>S<sub>8</sub>, and Fe<sub>6</sub>Ni<sub>3</sub>S<sub>8</sub>) were prepared by mixing of pure powders of elements and subsequent heating of the mixture in evacuated tubes. The methods of high-temperature X-ray diffraction, combined thermogravimetry, calorimetry, and mass spectrometry were used to study the structure, thermal expansion, and properties of pentlandites upon heating in an inert atmosphere (helium or argon) and air. Phase Transformations and temperature dependences of the unit cell parameters in the pentlandites were established. It was shown that the size of the elementary cells increased with growing Fe/Ni ratio in the pentlandites. Specific features of oxidation of the pentlandites during their continuous heating in air were determined. The research results can be used to develop pyrometallurgical technologies for nonferrous metallurgy and new ecologically friendly processes.

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P.S.B.1.

# MECHANISM OF PHOTOCATALYTIC DEGRADATION OF METOPROLOL IN AQUEOUS TITANIUM DIOXIDE SUSPENSION

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This study investigated efficiency of the photocatalytic degradation of metoprolol, a widely used  $\beta_1$ -blocker, in UV irradiated TiO<sub>2</sub> suspensions of Wackherr and Degussa P25. An attempt has also been made to identify the intermediate products formed during the photocoxidation process and suggest possible reaction pathways of the photocatalytic degradation. By examining the effect of ethanol as a hydroxyl radical ( ${}^{\bullet}$ OH) scavenger, it was concluded that the reaction with  ${}^{\bullet}$ OH was principally responsible for the photocatalytic degradation of metoprolol. After 240 min irradiation, the reaction intermediates were almost completely mineralized to CO<sub>2</sub>, H<sub>2</sub>O and the nitrogen was predominantly present as NH<sub>4</sub><sup>+</sup>. The degradation kinetics was monitored by LC-MS/MS, HPLC-DAD, IC and TOC analysis.

P.S.B.2.

### GROWTH AND MAGNETIC PROPERTIES OF InSb-MnSb EUTECTIC COMPOSITION

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One of the most actual problems of the spintronic for today is the search of the applicable materials. In order to do it is necessary to create new materials which provide effective injection of spin-polarized electron into semiconductor. The materials are bound to be ferromagnetic with the Curie point above room temperature and structurally compatible with common semiconductors. At the present time, there are no materials which meet the conditions in full. Mn-doped  $A^{III}B^V$  semiconductors (diluted magnetic semiconductors) are considered as promising materials for spintronics. The disadvantage of these materials is the low Curie temperature which is much lower than room temperature.

The InSb manganese doped alloys prepared with high speed of cooling are ferromagnetic with  $T_{\rm C}$ =580 K. The nature of the ferromagnetism of these compounds is determinated by the manganese antimonite nanoclusters. By the atomic force microscopy the average size of there nanoclusters was 24 nm. The magnetic clusters MnSb were also observed into poly- and monocrystalline samples and films of indium antimonide. The InSb manganese doped alloys can be used as materials for spintronic if they have constant composition and regular structure that provides the reproducibility of functional properties. The constant chemical composition can be achieved by using the InSb-MnSb eutectic and the regular structure can be achieved by the directional crystallization of this eutectic.

The coordinates of eutectic (6.5 mol% MnSb, Tm = $513^{\circ}$ C) of the InSb-MnSb phase diagram were determined by the complex of physical-chemical methods. The eutectic compositions were grown by Bridgman technique and were consisted of the monocrystalline InSb matrix oriented by direction [110] and monocrystalline faceted needles MnSb. The diameter of MnSb needles decreased from 20 to 3  $\mu$ m when the rate of crystallization varied from 0,2 to 2,5 mm/h. The eutectic composition had significant anisotropy of electroconductivity. The resistivity of the samples across the direction of the needles was 4-5 times higher (at low temperatures) and with increasing temperature 2-3 times higher, than along MnSb needles. The eutectic composition was magnetosensitive with Curie point 600 K. It can be used as a substrate material for ferromagnetic-semiconductor heterostructures.

P.S.B.3.

# ELECTRON STRUCTURE AND OPTICAL PROPERTICS OF $Gd_3Ga_5O_{12}$ GARNET DOPED WITH Tb

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Rare-earth doped gadolinium gallium garnet (Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub>) has attracted much attention as important material for application in many optical devices. Recently, the nanostructure materials are considered as potentially useful for many technological applications. This paper presents the results of electron structure and spectral-luminescent properties of pure and Tb<sup>3+</sup> doped Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> nanopowders prepared by a co-precipitation method. Analysis of diffractograms of the nanopowders showed that the minimum calcinations temperature that allowed getting a single garnet phase is  $T \sim 750^{\circ}$ C. An average crystalline size of powders is about 35-47 nm. The surface microstructure was observed by using an atomic force microscope Solver P47H-PRO. The luminescence transition  ${}^5D_4 \rightarrow {}^7F_i$  (green emission) is dominated at the X-ray and photo excitation of nanosized  $Gd_3Ga_5O_{12}$  doped with  $Tb^{3+}$ . The influence of the crystalline size and preparing condition on the luminescence properties of Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> is discussed. High-energy spectroscopy has been used to study the electron structure of the investigated rare-earth doped gadolinium gallium garnet (Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub>). The calculations of electron energy bands E(k) and partial DOS for compounds were performed by the semi relativistic linear muffin-tin orbital method without considerations of spin-orbit interactions. Effective filling numbers of electrons in different bands of components in garnet Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> been calculated. Between the experimental and calculated X-ray emission spectra garnet Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> good agreement has been obtained.

P.S.B.4.

#### CRYSTAL GROWTH RATE IN Y<sub>15</sub>Ba<sub>2</sub>Cu<sub>3</sub>O<sub>5</sub> WITH CeO<sub>2</sub> ADDITION

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Top-Seeded Melt-Growth (TSMG) process is technology used for production of the  $YBa_2Cu_3O_7$  (Y123) high temperature superconductors in the form of single-grain (single-crystalline) bulks. The TSMG process involves heating of the pressed Y123 powder (with addition of  $Y_2O_3$  to form excess of Y211 particles or direct addition of Y211 powder) to a temperature above that of the peritectic decomposition (incongruent melting) of the Y123 phase  $(T_{pY123}=1019^{\circ}C$  in air):

$$2(YBa_2Cu_3O_{7-\delta})(s) = Y_2BaCuO_5(s) + Ba_3Cu_5O_v(l) + zO_2(g).$$
 (1)

At this temperature, samples nearly retain their original shape. During slow cooling, the Y123 crystal (also called single-grain or single-domain) grows epitaxially from the seed, located at the top surface of the cylindrical sample, from an undercooled mixture of Y211 particles and a melt. Quality of growing crystal depends also on the level of undercooling below peritectic temperature,  $\Delta T$ , and consequent on growth rate, R. In this contribution we show the results of experimental measurements of growth rate, R, in the Y<sub>1.5</sub>Ba<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub> system with CeO<sub>2</sub> addition (for refinement of Y211 particles) in the c- and a-crystal direction in the temperature range 989 -998. The samples with a nominal composition Y<sub>1</sub>5Ba<sub>2</sub>Cu<sub>3</sub>O<sub>3</sub> with 1wt%CeO<sub>2</sub> additions were prepared in air in a chamber furnace. YBa2Cu3O7, Y2O3 and CeO2 powders were mixed and milled in appropriate amounts and uniaxially pressed into the cylindrical pellets of 20 mm in diameter. The samples were treated in a chamber furnace in air. The macrostructure of the sample surface was done by a stereo microscope. The sample cuts along the cylinder axis were prepared for microscopic analyses by grinding and polishing. The microstructure details were analysed under polarised light observation and by scanning electron microscopy with EDAX microanalyses. Measured crystal growth rate is anisotropic and the R<sub>a</sub>/R<sub>c</sub> ratio depends on undercooling. Smaller undercooling produces crystals with flat growth font and uniform fine subgrain structure while higher undercooling leads to disturbances of growth front and steps appearance on growing crystal. This is apparently responsible for higher crystal misalignments caused by subgrain formation. However, at higher growth rate also smaller Y211 particles are trapped in to growing Y123 crystal. The optimum undercooling is proposed for the Y123 crystal growth in the system studied.

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P.S.B.5.

### TEMPERATURE OF SELFNUCLEATION IN Y<sub>1.5</sub>Ba<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub> WITH CeO<sub>2</sub> ADDITION

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The  $YBa_2Cu_3O_7$  (Y123) high temperature superconductors in the form of single-grain (single-crystalline) bulks with trapped fine submicron  $Y_2BaCuO_5$  (Y211) particles are progressive materials which have practical applications at 77K where no equivalent can be found. The mostly used technology for production of this material is so called Top-Seeded Melt-Growth (TSMG) process. The TSMG process involves heating of the pressed Y123 powder (with addition of  $Y_2O_3$  to form excess of Y211 particles or direct addition of Y211 powder) to a temperature above that of the peritectic decomposition (incongruent melting) of the Y123 phase ( $T_{0Y123} = 1015^{\circ}C$  in air):

$$2(YBa_2Cu_3O_{7-\delta})(s) = Y_2BaCuO_5(s) + Ba_3Cu_5O_v(l) + zO_2(g). (1)$$

At this temperature, samples nearly retain their original shape. During very slow cooling, the Y123 crystal (also called single-grain or single-domain) grows epitaxially from the seed, located at the top surface of the cylindrical sample, from an undercooled mixture of Y211 particles and a melt. Important point of this epitaxial growth is the requirement to growth the sample below the temperature of heterogeneous nucleation of the used seed ( $T_{HN}$ ) and above the temperature of self-nucleation ( $T_{SN}$ ) of Y123 phase. In this contribution we show the results of experimental estimation of  $T_{SN}$  in the  $Y_{1.5}Ba_2Cu_3O_x$  system with CeO<sub>2</sub> addition (for refinement of Y211 particles) as well as microstructural features related to the solidification conditions. The microstructure after cooling from isothermal dwells in the temperature range 984 - 995°C was analysed. It is shown that blocky  $YBa_2Cu_3O_{7.\delta}$  crystals were self-nucleated and grown during isothermal dwells below 988°C and spheroidal multicrystals were formed during cooling from isothermal dwells at higher temperatures. The symmetrical and radial small angle  $YBa_2Cu_3O_{7.\delta}$  crystal branches of spheroids grow in the [100] crystal direction. These results enable deeper understanding of crystallization process of these important superconducting materials.

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P.S.B.6.

### OPTIMIZATION OF HEAT TREATMENT AND ITS INFLUENCE ON CORROSION BEHAVIOUR OF AZ61 MAGNESIUM ALLOY

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The influence of solution heat treatment on corrosion behaviour and mechanical properties of AZ61 magnesium alloy prepared by squeeze casting was evaluated. Experimental material was subjected to solution heat treatment at 380°C for various periods of time with subsequent water quenching. Metallographic analysis and tensile tests were proposed for assessment of optimum conditions of heat treatment. A temperature of 380 °C and an annealing time of 6 hours at the temperature were found to be optimal. Corrosion behaviour of both conditions, ascast (F) and solution heat treated (T4) was evaluated through neutral salt spray test and electrochemical impedance spectroscopy method. Corrosion rate was established on the basis of mass losses, the corroded surfaces were analyzed using SEM. Polarization resistance as a basic electrochemical characteristic was evaluated by the electrochemical impedance spectroscopy. Electrochemical characteristics were determined after various exposure times (from 5 mins up to 168 hours) in 0.1M NaCl solution. Mechanical properties of AZ61 magnesium alloy were improved by heat treatment while corrosion resistance in as-cast condition was higher than inT4 condition due to presence of  $\gamma$  phase that acts as barrier in process of corrosion.

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P.S.B.7.

### IMPACT ANALYSIS OF SHOT PEENING OF ALUMINIUM ALLOY AW 6082 ON THE FATIGUE PROPERTIES

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The influence of shot peening on fatigue resistance of the wrought AW 6082 aluminium alloy was investigated in the very high cycle region. Specimens with as machined and shot peened surfaces were subjected to high frequency fatigue loading ( $f \approx 20 \text{ kHz}$ ,  $T = 20 \pm 3^{\circ}\text{C}$ , R = -1). Shot peening process led to the formation of compressive residual stresses in the surface layer and effectively improved the fatigue resistance. The fracture surfaces after fatigue loadings were evaluated by fractographical analyses using light stereo microscope and scanning electron microscope. There were evaluated the initiation stage of the fatigue process, propagation of fatigue cracks in the fatigue strength and general morphology of the fracture surfaces. The tests results showed that the fatigue strength for shot peened specimens is much higher than the one for as machined specimens in the all investigated range of cycles.

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P.S.B.8.

#### REAGENT OXIDATION OF INTERMETALLIDE NbAla

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The interaction of intermetallide NbAl<sub>3</sub> with Na and Ca carbonates was investigated by thermal, electron-probe microanalysis (EPMA) and X-ray analysis. The equilibrium compositions of reaction products and heat balance of processes calculated by thermodynamic analysis. Calcium carbonate begins to interact with NbAl<sub>3</sub> at 900°C which leads to the formation of Ca<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub> and Ca<sub>2</sub>AlNbO<sub>6</sub>. We established the following sequence of chemical transformations in the sodium carbonate–NbAl<sub>3</sub> system on air heating: Nb<sub>2</sub>O<sub>5</sub> and Al<sub>2</sub>O<sub>3</sub> first form which transform into NaNbO<sub>3</sub>, Na<sub>3</sub>NbO<sub>4</sub> and NaAlO<sub>2</sub>. The efficiency of this transformation increases above the melting temperature of sodium carbonate (above 850°C). Calculations of kinetic parameters (n, D, E) have confirmed that NbAl<sub>3</sub> oxidation with additives proceeds in some stages and is limited by the oxidizer diffusion. The oxidation process parameters were determined using an anisothermal kinetic method.

P.S.B.9.

#### MAGNETOCALORIC EFFECT IN NI-MN-GA BASED ALLOYS

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Materials with high magnetocaloric effect (MCE) have attracted considerable attention as a refrigerant for magnetic refrigeration. This study reports on the Ni-Mn-Ga alloys which seem to be promising candidates for application in magnetic cooling. These alloys show entropy change at the structural phase transition (SPT), at room temperature. The SPT and magnetic entropy change strongly depends on composition of the Ni-Mn-Ga alloys. The alloy composition can be controlled by the Mn/Ga ratio and the electron concentration (e/a). When one of these parameters was changed, different behavior of SPT temperature and entropy change has been observed.

P.S.B.10.

#### IMPEDANCE SPECTROSCOPY OF MULTIDOPED CERIA

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Ceria based nanopowders were prepared in two different ways by applying modifed glicine/nitrate (MGNP) and self propagating room temperature (SPRT) methods. Nanopowders differed in properties with particle size of SPRT powder being an order of magnitude lower in comparison with powders obtained by MGNP procedure. Two different compositions were sinthezed:  $Ce_{0.8}Nd_{0.01}Sm_{0.04}Gd_{0.04}Dy_{0.04}Y_{0.07}O_{2-\delta}$  and  $Ce_{0.8}Sm_{0.005}Gd_{0.005}Dy_{0.095}Y_{0.095}O_{2-\delta}$ , as well as pure ceria for comparison. Characterization of the powders was performed by impedance spectroscopy. The electrical conductivity increased from  $1.36 \times 10^{-6} \ Scm^{-1}$  to  $4.01 \times 10^{-3} \ Scm^{-1}$ , with the temperature increase from  $200^{\circ}C$  to  $450^{\circ}C$ , with step of  $50^{\circ}C$ .

P.S.B.11.

### MONTE CARLO ANALYSIS OF THE INFLUENCE OF DIFFERENT PACKAGING ON MOSFET ENERGY RESPONSE TO X-RAY AND GAMMA RADIATION

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Radiation sensing MOSFETs have found numerous applications as detectors or device components in radiation fields used in nuclear industry, medical applications and space research. Monte Carlo simulations of MOSFET energy response to X-ray and gamma radiation for different packaging were performed. The photon transport Monte Carlo software FOTELP-2K10 has been adapted to obtain the energy deposited in MOSFET structure with microscopic dimensions. Based on results of the energy deposited in MOSFET configuration, detector packaging was optimized. The energy response of different packaging would be more consistent in practical use as the small over-response and under-response will compensate each other for different energy of photon beams.

P.S.B.12.

### THE TOUGHNESS AND FATIGUE ANALYSIS OF Nd-Fe-B/EPOXY MAGNETIC COMPOSITES

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Magnetic composite materials based on Nd-Fe-B alloy are prepared by compression molding technique using different contents of magnetic particles. Thermosetting epoxy resin is used as a polymer matrix. Homogeneous distribution of magnetic particles in the polymer matrix is validated using Scanning Electron Microscope (SEM). The effect of reinforcements on fatigue crack growth parameters is analyzed using the high frequency resonant pulsator equipped with three-point bending clamp. The testing specimens of pure epoxy resin and composites containing 50 wt. % and 75 wt. % of magnetic filler are observed. The thermal properties and magnetic characteristics are examined by varieties of techniques including simultaneous Differential Scanning Calorimetric and Thermogravimetric Analysis (DSC/TGA) as well as SQUID magnetic measurements. Obtained results depict that the crack growth rate rises with increasing content of magnetic particles. Also, the mechanical and magnetic properties are increased, while the toughness and overall energy of impact are decreased with higher content of Nd-Fe-B filler.

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P.S.B.13.

# ELECTROCHEMICAL STUDY OF COMPLEX FORMATION BETWEEN SOME TRANSITION CATIONS AND N,N',N'',N'''-TETRAKIS(2-PYRIDYLMETHYL)-1,4,8,11-TETRAZACYCLOTETRADECANE

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Macrocyclic ligands have important role in ion transport across artificial and biological membranes and in understanding of some natural processes through mimicry of metalloenzymes. They were also successfully used in design of many ion-selective electrodes. The aim of this work was to examine complexation reactions of macrocycle N,N',N'', tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane with  $Cu^{2+}$ ,  $Co^{2+}$ ,  $Ni^{2+}$ ,  $Ag^+$  and  $Fe^{3+}$  ions using a conductometric method in acetonitrile and in an aqueous media by cyclic voltammetry. The conductance data show that the stoichiometry of the complexes in most cases is 1:1 (ML), while for  $Fe^{3+}$  ion, 2:3 ( $M_2L_3$ ) complexes are formed in solutions. The results obtained by this two techniques were compared with sensor behavior of ion-selective electrode based on N,N',N'', -tetrakis(2-pyridylmethyl)-1,4,8,11-tetraazacyclotetradecane as an ion carrier, in order to explain clearly nature of processes on sensor membrane itself.

P.S.B.14.

### ANALYSIS OF TERMALLY ACTIVATED PROCESSES IN COLD ROLLED AND ANNEALED NiAI BASED INTERMETALLIC STRIPS

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The influence of recovery and recrystallization processes on a structure and properties of cold rolled and annealed  $Ni_3Al$  intermetallic alloy were examined. The investigated material in a shape of fine grained strip was cold rolled up to 50% of thickness reduction and then annealed for one hour at temperature in range of  $300\text{-}1200^{\circ}C$ . The results of electric conductivity, longrange ordering parameter, hardness and static tensile test investigations were taken into consideration to analyze a course of recovery and recrystallization phenomena. The above mentioned parameters were referred to the changes of strip microstructure analyzed by quantitative SEM microscopy. It has been stated that the temperature of the  $Ni_3Al$  intermetallic strip full recrystallization start was approx.  $900^{\circ}C$  and that the course and intensity of recovery process strongly influence the final results of recrystallization.

Keywords: Ni3Al intermetallic strips, long-range ordering, cold rolling of intermetallics, recovery of ordered alloys, recrystallization of ordered alloys.

P.S.B.15.

# THERMAL STABILITY OF FeAI SINTERS STRUCTURE WITH ADDITION OF $\mathrm{Al}_2\mathrm{O}_3$ NANOMETRIC CERAMIC

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Addition of nano-ceramic in a form of alumina particles to FeAl intermetallic sinter is significant while the alloy is working at elevated temperature. To manufacture Fe40Al sinter with or without alumina nano-ceramic, commercial purity powders iron (99.9%), aluminum (99.5%) and nanometric  $Al_2O_3$  (99,5%) were used. Preliminary, iron and nano- $Al_2O_3$  composite powders were prepared by low-energy milling of iron powder with nanometric alumina powder in planetary mill. Next, the aluminum and iron powders (target material composition – Fe40Al) were mixed together with (Fe+ nanometric  $Al_2O_3$ ) composite powder to obtain powder mixture containing 0%, 0.5%, 1%, 1.5%, 2% or 5% volume addition of  $Al_2O_3$ . The obtained mixture of powders were formed by cold-consolidation at 300MPa pressure, preliminary sintered at 1050°C under 40MPa for 15 minutes in vacuum and finally heated at 1200 °C for 1 hour in argon atmosphere. Nano-composite sinters were than cyclically heated at 800 °C or 1000 °C in air atmosphere for 150h. The smallest value of FeAl grains equivalent diameter (ECD) after full time of heating was observed for Fe40Al + 1% vol. nano- $Al_2O_3$  sinter, and it stands 4.2 $\mu$ m or 4.4 $\mu$ m for 800°C and 1000°C respectively, versus 3.5 $\mu$ m of initial sinter grain size. Additionally, the best oxidation resistance for Fe40Al + 1% vol. nano- $Al_2O_3$  was stated.

Keywords: Fe-Al sinters, nano-composite materials; nano-alumina, thermal stability.

P.S.B.16.

### STRUCTURE CHANGES AT CRYSTALLIZATION OF Zr<sub>57</sub>Ta<sub>8</sub>Nb<sub>2,5</sub>Cu<sub>13,4</sub>Ni<sub>11,1</sub>Al<sub>7,5</sub> AMORPHOUS ALLOY

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Structure changes at heating of Zr<sub>57</sub>Ta<sub>8</sub>Nb<sub>2,5</sub>Cu<sub>13,4</sub>Ni<sub>11,1</sub>Al<sub>7,5</sub> amorphous alloy has been studied both by means of X-Ray diffraction and differential scanning calorymetry methods. Sample of Zr<sub>57</sub>Ta<sub>8</sub>Nb<sub>2,5</sub>Cu<sub>13,4</sub>Ni<sub>11,1</sub>Al<sub>7,5</sub> was obtained by mixing of pure elements of high purity, melting and than quenching from liquid state in order to produce the amorphous phase (Johan Otto GmbH equipment). Intensity curves, obtained for room temperature and at heating to 690 and 750 K, diffraction pattern was also obtained for annealed at *T*=725 K and then quenched sample. It is shown, that heating of amorphous alloy is accompanied by formation of NiZr<sub>2</sub> intermetallic and quasicrystalline phase. Before formation of quasicrystalline phase, amorphous alloy transforms its structure in order to be more close to structure of nanocrystals still at lower temperatures. Such behavior also supposes the transformation of cluster structure with temperature change.

Keywords: quasicrystals, amorphous alloys; heat treatment; structure modification.

P.S.B.17.

### FORMATION OF THE SOLID SOLUTION $Cr_{0.9}Ta_{0.1}Si_2$ IN THE COURSE OF SOLID PHASE INTERACTION

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In order to clarify the regularities of the solid solution  $Cr_{0.9}Ta_{0.1}Si_2$  formation, study of the mechanism and peculiarities of its formation from micron–sized powders of initial components has been carried out in the temperature range 400-1300°C at two-hour isothermal exposure. The interaction of powders of individual elements begins at 600°C, when the lower tantalum silicide. At 700°C formation of the tetragonal  $Cr_5Si_3$  phase, isostructural with  $W_5Si_3$ , is observed in the interaction products, which exists to 1100°C. In the temperature range 800-1000°C the products of solid phase interaction contain tantalum silicide  $Ta_5Si_3$ , isostructural with  $W_5Si_3$  and  $Nb_5Si_3$ . Formation of higher silicide phases of tantalum and chromium starts at 900°C. The mechanism of formation of the solid solution  $Cr_{0.9}Ta_{0.1}Si_2$  includes such stages as formation of tantalum and chromium disilicides at 900°C and their mutual solution (both  $CrSi_2$  in  $TaSi_2$ , and  $TaSi_2$  in  $CrSi_2$ ) at 1100°C confirmed by the increase in the lattice parameter of  $TaSi_2$  compared to their equilibrium values. Finally, in the temperature range 1100-1300°C, the formation of the solid solution  $Cr_{0.9}Ta_{0.1}Si_2$  occurs.

Prior mechanical activation of initial components (chromium, tantalum, silicon) significantly affects solid phase interaction compared to micron–sized powders, namely decreases the temperatures of both the start and completeness of the interaction by 300-400°C Herein the mechanism of solid solution formation remains the same as in the case of micron–sized powders, that is, through successive stages of formation of individual silicide phases from lower to higher silicides with subsequent dissolution of tantalum disilicide in the lattice of chromium disilicide. Low temperature synthesis of prior activated initial components permits one to produce a nanosized powder of solid solution with high enough reproducibility of the element composition.

P.S.B.18.

### MODELLING OF ELECTRONS AND HEAVY PARTICLES IN PURE H2 DISCHARGE

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We calculated  $H_{\alpha}$  emission profiles from Townsend discharges in pure hydrogen between two parallel electrodes focusing on details of heavy particle interaction with the cathode surface. The basic data were provided by A. Phelps [1]. Monte Carlo simulation technique employing null collision method was used to follow electrons and heavy particles between collisions with  $H_2$  or with surface for the conditions of a high electric field (*E*) to gas density (*N*) ratios *E/N*. Trajectories of reaction fragments are followed after the collision until their neutralization or thermalization down to the threshold of  $H_{\alpha}$  excitation. For the conditions of Phelps and Petrović's experiment [2] we obtained spatially resolved emission profiles and Doppler broadened line profiles. Intensity of Doppler profile wing showing  $H_{\alpha}$  emission of particles emerging from the cathode direction is obtained assuming that the reflection coefficient of fast H atoms depends on the incident angle and on energy of the incident particle. Some effects of collision dynamic of heavy particles with  $H_2$  on Doppler broadened profile are discussed. Fast neutral etching is the leading candidate to reduce charging induced damage in etching of high aspect ratio holes in dielectrics. It also reduces the roughness of etched surfaces allowing extension of plasma related technologies below 22 nm.

- [1] A.V. Phelps, PHYSICAL REVIEW E 79, 066401 (2009).
- [2] Z. Lj. Petrović and A.V. Phelps, PHYSICAL REVIEW E **80**, 066401 (2009).

P.S.B.19.

# TEMPERATURE AND PRESSURE DEPENDENCE OF RAMAN SPECTRA IN CRYSTALLINE GeS<sub>2</sub>, AND GeSe<sub>2</sub>

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Germanium dichalcogenide systems, amorphous and crystalline, have been studied for many years because of their interesting physical properties and many potential applications. Here we report pressure and temperature effects on the Raman active phonons in layered molecular crystals GeS<sub>2</sub> and GeSe<sub>2</sub>. The Raman spectra have been investigated as a function of temperature (18 – 300 K), and as a function of hydrostatic pressure, up to 2.5 GPa, at room temperature. Results of the effect of pressure on the phonon frequencies were analyzed in the usual way (using frequency dependence of the Grüneisen parameter,  $\gamma_i(v_i)$ ). The correlation between the pressure–induced relative change and mode frequency is in accordance with previous findings on molecular crystals;  $\gamma_i(v_i)$  is very large and remains constant for the external modes but rapidly drops as  $\gamma_i(v_i) \sim v_i^{-2}$  in the internal mode region. The influence of the temperature on the phonon frequencies is presented in the form of the logarithmic temperature derivative,  $(1/v_i)(dv_i/dT)$ . The simple scaling law.  $(1/v_i)(dv_i/dT) \sim v_i^{-1}$  holds both for internal and external modes.

P.S.B.20.

# CHANGES IN MICROSTRUCTURE AND MECHANICAL PROPERTIES OF Ni-25%Mo-8%Cr ALLOY AFTER LONG TIME ANNEALING AT 650 °C

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Ni-25%Mo-8%Cr alloy known under its commercial name Haynes 242, is an agehardenable superalloy. It is developed for applications requiring a combination of good corrosion resistance, good strength and a low thermal expansion coefficient. It is used for various components of gas turbine engines (seal and containment rings, fasteners, casings, rocket nozzles etc.). Such a broad application range is also related to its good forming and welding characteristics. Good mechanical properties are achieved from a fine dispersion of metastable Ni<sub>2</sub>(Mo,Cr) ordered body centered orthorhombic (Pt<sub>2</sub>Mo-type) precipitates in a face centered cubic y matrix. Standard heat treatment which consist of solution and 24 to 72h aging at 650°C, produces very small domains of the Ni<sub>2</sub>(Mo,Cr) phase. The aged alloy exhibits almost double yield strength over the annealed condition. Recent calculations of phase stability in the Ni-Mo-Cr system by the CALPHAD approach predict stability of Ni<sub>2</sub>(Mo,Cr) phase at temperatures below 620°C for some alloy compositions. Though a long term thermal stability of this phase is a critical issue in applications of this alloy at elevated temperatures, its behavior at elevated temperatures has not been investigated extensively. The aim of the study was the characterization of the microstructure and measurement of tensile properties of Haynes 242 alloy which was deformed by cold rolling and further subjected to long-term annealing at 650°C for different times.

P.S.B.21.

# THE DETERMINATION OF INERTIA MOMENTS OF DETAILS WITH COMPLEX SHAPE

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In this study is treated the problem of the accuracy of inertia moments of bodies with complex shape, performing a circular motion. The importance of the accuracy of calculating inertia moments of the masses, directly affects in the values of oscillation frequency and the level mechanical vibrations of system. This does, to accurate the areas of resonance and amplitude of oscillation. The reducing the level of vibrations of the system, achieved by changing this parameter. As a case study for the calculation is taken main detail of the internal combustion engine, the crankshaft. For this case is used the theoretical method, which calculates the moment of inertia by the working drawing. In fact in practice, the completed details change with the form given in drawing theoretical, because affect the technological tolerances of production and dynamic balancing process. For this reason and irregular distribution of the material used experimental methods. For this case is used the hanging method, which is a simple method to apply and consists in the hanging of detail in two elastic yarn through a device, which designed and produced easily. Through the measurement of time of 100 oscillations, is determined the average period for 3 measurements and from this extracted value of the moment of inertia of detail. From experimental measurements carried out for 4 crankshafts has shown that the values of moments of inertia determined experimentally are about 7% smaller than its theoretical value and change by 4% from one detail to another. This method can easily be used for other details that make a circular motion, which affect in the oscillation of the system in torsion, such as ship propellers, which during the repairs can be exchange and it affects in the travel comfort.

Keywords: inertia moments, ship, frequency, parameter, detail.

P.S.B.22.

# PECULIARITIES OF THE MoSi<sub>2</sub>-CrSi<sub>2</sub> SOLID SOLUTION FORMATION DEPENDING ON THE CONDITIONS OF SOLID PHASE SYNTHESIS

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Materials and coatings oriented at operation in oxidizing media at high temperature are of great interest as heaters, sensors, protective multifunction coatings to be used over the temperature range 1000-1800 °C in chemical and related areas of industry as well as in aircraft and space engineering. Modern technologies require novel materials and coatings which possess a unique complex of physical and chemical properties. The features of the solid solution  $(Mo_{0.9}Cr_{0.1})Si_2$  formation through solid-phase synthesis have been investigated depending on the morphology, dispersity and defectiveness of initial components and the conditions of highenergy mechanical processing. It was established that a solid solution is formed due to reaction diffusion through intermediate stages of formation of solid solutions on the basis of lower and higher phases of molybdenum silicide followed by their interaction. Preliminary mechanical activation significantly affects the solid-phase interaction: it reduces the temperature of both the beginning and end of the interaction. Under milling in a high-energy planetary mill AIR (acceleration 25 g) for 90 min, nuclei of the high-temperature unstable hexagonal phase, β-MoSi<sub>2</sub>, are formed, which significantly affects the character of the interaction process by reducing temperature of the beginning and end of the interaction by 300-600 °C and thus makes it possible to produce non-milled nanosized powders of solid solution. Formation of a solid solution under heat treatment due to the high reactivity of the initial mixture is accompanied with simultaneous formation of solid solutions based on two modifications (tetra- and hexagonal) of the higher molybdenum silicide with subsequent allotropic transformation of the high-temperature unstable hexagonal β-MoSi<sub>2</sub> phase into the low-temperature tetragonal phase, α-MoSi<sub>2</sub>.

P.S.B.23.

### INSTRUMENTED INDENTATION OF WC-Co CEMENTED CARBIDES

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The instrumented indentation offers new possibilities in the hardness measurement of advanced ceramics in the range of nanoindentation and measurement of hardness of thin coatings and phases and grains with small size in the microstructure of bulk composites and/or coatings. However, many aspects are not clear, for example; the relationship of conventional and instrumented hardness, the source of the scatter in hardness measurement, etc. The instrumented indentation technique offers a number of new testing methods, especially indentation fatigue and indentation creep, which are underdeveloped until now.

Statistical indentation of heterogeneous materials, the so called "Grid-Indentation Technique (GID)" is often applied to various composites. It is realized by carrying out a large array of nanoindentation in multi phase material and mechanically active phases are statistically identified.

This work is focused on statistically identification of mechanically active phases in WC - Co and on influence of microstructure on indentation fatigue in WC - Co composites.

Instrumental indentation with Berkovich indenter was used for nano/micro indentation hardness test in the load interval from 3 mN to 200 mN in single load – unloading regime. The indentation hardness  $H_{\rm IT}$  and elastic modulus  $E_{\rm IT}$  values have been calculated. So called grid indentation technique (GIT) was applied, which assumes using large array of indents and statistical evaluation of the resulted hardness and elastic modulus. Indentation fatigue experiment has been also performed for selected systems (systems 35 and 60). The specimens were indented with maximum load of 25 mN, 50 mN, 100 mN and 200 mN, than reloaded to 50% and repeatedly re-loaded in 100 cycles with the speed of 1000 mN/min.

P.S.B.24.

# MICROSTRUCTURE AND MECHANICAL PROPERTIES OF FRICTION STIR WELDED OF A 7042 ALUMINIUM

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This research characterizes the changes in the microstructure that occur in friction stir welded extrusions of a novel 7042 aluminum alloy. The 7042 alloy, belonging to the Al-Zn-Mg-Cu group, contains small additions of zirconium and scandium. The addition of scandium brings about the formation of minute coherent  $Al_3(Sc,Zr)$  precipitates which hamper recrystallization during hot extrusion. This results in preserving the deformed microstructure of highly elongated primary grains in the extruded material. Though intensive recovery occurs during extrusion, a fairly large number of dislocations is present in the microstructure of the base material Friction stir welding is a joining technology which does not involve material melting, other, the joined material is heated due to friction to high temperature but below the melting point. The temperature increase is high enough to make significant changes in the microstructure within the weld and its vicinity. Since the examined material is an age-hardenable one, the changes in morphology of the hardening phase were of particular interest. The changes in microstructure were investigated by light microscopy (OM), transmission electron microscopy (TEM) and scanning electron microscopy (SEM).

P.S.B.25.

# CORROSION RESISTANCE OF FRICTION STIR WELDED 7XXX SERIES ALUMINUM ALLOYS

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Aerospace structures are often subjected to adverse environmental conditions and deteriorate during their service life. Thus corrosion investigations of materials are very important. Aluminum alloys offer a wide range of properties that are particularly advantageous for aerospace applications. Aluminum alloys of 7xxx series combines superior mechanical performance with excellent resistance to corrosion. However, application of these alloys is limited due to problems associated with their welding. In general, the aluminum alloys are classified as non-weldable. Due to the inability of joining these alloys by conventional fusion welding, research into the application of a novel joining technique - friction stir welding (FSW) – has been undertaken. This research addresses the characterization of the corrosion resistance in friction stir welded 7xxx series aluminum alloys extrusions.

P.S.B.26.

# STRUCTURE AND PROPERTIES OF Ti(C,N,O) THIN FILMS DEPOSITED BY PLD TECHNIQUE ON POLYURETHANE SUBSTRATE

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In the paper the results of investigations of Ti(C,N,O) thin films deposited on polyurethane substrate for biotechnological applications are presented. The thin films were deposited using PLD (Pulsed Laser Deposition) technique. Nd:YAG pulsed laser with 1-1,7 [J/cm²] energy density was used. The paper presents PLD process parameters optimization, as well as the morphology, microstructure and chosen properties of thin films. Ti(C,N,O) films morphology was characterized by AFM (Atomic Force Microscopy) and SEM (Scanning Electron Microscopy) methods. Microstructure was investigated using TEM (Transmission Electron Microscopy) and HREM (High Resolution Electron Microscopy) techniques. Chemical composition of obtained films was studied by EDS (Energy Dispersive Spectroscopy) and XPS (X-ray Photoelectron Spectroscopy) and phase composition was investigated by XRD (X-ray Diffrction). The paper presents also the results of adhesion to the substrate measurements (nanoscratchtester) and nanohardness measurements. The results of investigations show, that the thickness of deposited thin films is about 40 nm. The cracks and delamination of titanium oxide films were not observed. Very interesting is that high deformation of elastic polyurethane substrate do not cause delaminations and cracks appearance in the ceramic thin films.

P.S.B.27.

# PROCESSING AND CHARACTERIZATION OF COMPOSITE POLY (METHYLMETHACRYLATE)-BISMUTH-SILICON-OXIDE

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Polymer composite PMMA-Bi $_{12}$ SiO $_{20}$  has been chosen because of it's potential as material for production of scintillating polymer optic fibers (POF). Samples of pure PMMA and composite with 0.5 mas% of Bi $_{12}$ SiO $_{20}$  (BSO) powder were made using laboratory mixing molder. Characterization of starting components as well as composite was performed using FTIR. Measurements of refraction indices using spectroscopic ellipsometry method have shown that refraction index of composite material with BSO powder has higher value compared to pure PMMA. Results of tensile testing have shown increase of Young's modulus with the implementation of BSO. Dynamic-mechanical analysis results revealed increase of storage modulus, loss modulus and glass transition temperature ( $T_g$ ) of the polymer composite with the addition of the powder.

P.S.B.28.

# ON-LINE AND OFF-LINE PYROLYSIS FOR DETERMINATION OF POLY(VINYLPYRROLIDONE) IN WASTEWATER SAMPLES

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In contrast to the very intensive study of low molecular weight organic pollutants occurring in wastewaters and river waters, the pollution with synthetic polymers has received by far less attention. Poly(vinylpyrrolidone) (PVP) is a widely used water soluble polymer whose occurrence in wastewaters is likely. PVP is intensively used in the pharmaceutical industry as a binder in many tablets and in the production of one of the most important disinfectants, PVPiodine. PVP also has application in detergents and in personal care products such as shampoos and hair gels. The PVP is presumed to be detected in the polluted water samples as a result of its very frequent usage and suggested environmental stability. However, an appropriate method for its identification and quantification in environmental samples is still lacking. In this work online and off-line pyrolysis, connected with gas chromatography (GC) was applied for detection and quantification of PVP in wastewater samples. Pyrolysis of commercial PVP, spiked water samples and wastewater samples was performed in both on-line conditions (5 s at 750 °C) and off-line conditions (in a tube furnace, 1 h at 500 °C), in order to cause rapid polymer fragmentation into volatile products - compounds capable of being analyzed using GC. In online technique, the pyrolysator was directly connected with GC column, while in off-line conditions degradation products were trapped in dichloromethane and after that quantified by GC-FID analysis. The concentration of PVP was calculated on the basis of the main pyrolytic product, N-vinylpyrrolidone (NVP) in both on-line and off-line experiments. Very good linear correlations between initial amounts of PVP and released amounts of NVP were obtained. The second standard curve, which correlated the weight of NVP with the ratios of the areas of NVP peak and internal standard peak, was used for calibration in off-line conditions. The internal standard was 4-tert-butylcyclohexanone (BCH). The concentration of PVP in wastewater samples was between 2.5 and 2.9 mg/dm<sup>3</sup>. Main drawbacks of the on-line systems were memory effects caused by the presence of non-volatile compounds in the aerosol produced by pyrolysis, deterioration of GC column and poor chromatographic behavior of polar compounds. Although more time consuming, off-line pyrolysis was successfully used in order to overcome these problems, Furthermore, continuous-flow off-line pyrolysis coupled to GC-FID is very suitable for PVP detection in wastewater samples because the optimal size of the sample can be easily adjusted prior to GC analysis and the internal standards can be used in order to improve accuracy of quantitative determination of pyrolytic products, which is not readily attainable with on-line pyrolytic systems.

P.S.B.29.

# LOW-CYCLE FATIGUE OF THERMALLY-CYCLED CARBON-EPOXY COMPOSITE

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Investigation of low-cycle fatigue of composites is of vital importance for the design of structural components. In this study, the effects of thermal cycling on low-cycle fatigue behavior of carbon-epoxy laminate are investigated in a purely bending mode at strain ratios of -1 and 0.1. It is found that a very small increase in the plastic strain amplitude  $\Delta\varepsilon_p$  catastrophically shortens the fatigue life of the composite determined as a number of cycles corresponding to 0.9 of the initial force. For example, in case of reversible loading, an increase in the plastic strain amplitude from 0.002 to 0.003 corresponds to lifetime decrease by one order of magnitude (from  $10^4$  to  $10^3$  cycles). The preliminary thermal cycling of the composite at the temperature varied from  $180^{\circ}$ C to  $-195^{\circ}$ C shortens the fatigue life in comparison to the reference at small plastic strain amplitudes.

P.S.B.30.

# TENSILE PROPERTIES OF NOVEL POLYCARBONATE-BASED POLYURETHANE ELASTOMERS

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Novel polyurethane elastomers based on aliphatic polycarbonate macrodiol and aliphatic diisocyanate (PC-PU), as well PC-PU nanocomposites filled with organic-modified clays have been synthesized and studied. They have distinctly segmented structure resulting in strong physical rubbery network. In previous studies, the PC-PU were found to possess superior mechanical properties. In this paper, mainly static tensile properties under various conditions are focused. This research is kindly supported by Grant Agency of the Czech Republic (Czech Science Foundation, project no. P108/10/0195).

P.S.B.31.

# INFLUENCE OF THERMAL TESTS ON PHASE TRANSFORMATION IN NANOSTRUCTURED CERAMICS ${\rm ZrO_2(MgO)}$

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It has been studied an influence of thermal tests at cooling in water from temperature of  $1000\,^{\circ}\text{C}$  on phase transformations in nanostructured ceramics based on  $\text{ZrO}_2$ , partially Mg-stabilized. Ceramics has a different amount of magnesia in solid solution, and, as consequence, has different amount of high- and low-temperature modifications of zirconia. It have been shown that while of thermal tests number is increase there was a zirconia destabilization, however, ceramics has a high resist for thermal shock.

P.S.B.32.

# STRUCTURE AND PROPERTIES OF ZIRCONIA-ALUMINA CERAMICS BASED ON OXIDE-HYDROXIDE MIXTURES

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The structure of zirconia-alumina ceramics based on oxide-hydroxide mixtures was studied. It was shown that the porosity in  $ZrO_2$  ceramic depends on the type of doping oxide – for yttria oxide it's 40% and for magnesia oxide – 5%. It has been shown that the increasing of  $Al_2O_3$  powder content led to the decreasing of porosity volume up to 25 %. In the ceramic sintered from  $ZrO_2$ -Al(OH)<sub>3</sub> mixtures the dependence of porosity vs. alumina oxide content was steadily increasing from 5 up to 20 %. It was explained that porosity volume increased due to the decomposition of Al(OH)<sub>3</sub>. The mechanical properties of sintered materials were studied.

P.S.B.33.

# DETERMINATION AND APPLICATION OF MATERIALS FOR AUTOMOTIVE TURBOCHARGERS

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In this paper, are presented the results of research work on innovation project which are some of materials used to produce proper alternative parts service kit turbocharger for automotive industry, and how modeling and material selection in the CAD/CAM software in order to ensure successful production of service parts. We also found that some same parts of the service sets can be artifacts of copper and silicon nitride. This paper also presents comparison of these characteristic materials and advantages and disadvantages of using these materials that can be made the same replacement parts.

P.S.B.34.

# THE CORELATION BETWEEN THE CHANGE IN THE DENSITY OF FREE ELECTRONS AND THE RELATIVE MAGNETIC PERMEABILITY OF THE AMORPHOUS ALLOY $FE_{37.5}NI_{17.5}CR_5CO_{15}SI_{10}$ UNDER THE INFLUENCE OF HEAT ACTION

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The object of investigation was the influence of heat action on structural changes in the nanostructure of the alloy Fe<sub>37.5</sub>Ni<sub>17.5</sub>Cr<sub>5</sub>Co<sub>15</sub>Si<sub>10</sub> at the temperatures ranging from room temperature to 600°C.The conducted thermomagnetic measurements helped to establish that magnetic properties of a cooled of alloy sample changed upon multiple heating procedures. Upon heating to 300 °C, the magnetization of the cooled off sample increased by 12% in relation to that of the original alloy sample. Upon another heating to 360 °C, the magnetization of the cooled off sample increased by approximately 20% in relation to that of the original alloy sample. Upon further multiple heating procedures, it was determined that heating to 420 °C brings about the decrease in the magnetization of the cooled off alloy sample by 5%. Heating to 600 °C brings about the decrease in the magnetization of the cooled off sample by 40% in relation to that of original sample. This decrease is caused by the crystallization of the examined sample. The method of measuring TEMF (thermo-electromotive force) of the thermopair Cuamorphous alloy Fe<sub>37.5</sub>Ni<sub>17.5</sub>Cr<sub>5</sub>Co<sub>15</sub>Si<sub>10</sub> helped to establish that the temperature coefficient of TEMF direction changed upon every period of cooling off. The change of the temperature coefficient of TEMF direction was caused by the change in the density of free electron carries under the influence of heat action.

P.S.B.35.

# CHARACTERIZATION OF IRON-COBALT BASED ALLOYS PROCESSED BY PIM ROUTE

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Powder injection molding (PIM) is technology which can offer manufacturing parts with complex geometries. Iron-cobalt based alloys exhibit high saturation magnetic induction as well as high Curie temperature. Therefore, ferromagnetic parts with complex shapes for high temperature applications can be produced as iron-based alloys by PIM route.

We have characterized Fe49Co49V2 alloys samples produced by PIM. The feedstock for powder injection molding was prepared by mixing starting FeCoV powder with a low viscosity binder. Green samples were subjected to solvent debinding and subsequent thermal debinding followed by sintering. Sintering was performed during 3.5 hours: from 1370  $^{\rm o}$ C to 1460  $^{\rm o}$ C in hydrogen atmosphere or from 1330  $^{\rm o}$ C to 1400  $^{\rm o}$ C in vacuum.

Electrical, mechanical and magnetic properties were investigated as a function of sintering atmosphere and sintering temperature. In addition, magnetic properties were analyzed as frequency dependent and obtained results were compared with other iron-cobalt based alloys prepared by conventional methods.

P.S.B.36.

# PLASTIC DEFORMATION MODELING OF SINGLE CRYSTALS WITH THE NaCI-TYPE LATTICE

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Process of plastic deformation of single crystals is well described phenomenologically and it is actively investigated experimentally. Hardening, weakening and creep in single crystals in many cases are determined by the processes in dislocation subsystem. Movement of dislocations is the major process during a non-steady creep. In experiments and modeling KCl and NaCl single crystals with dimensions  $3\times6\times10$  mm and initial density of dislocations  $\sim 10^5$  cm<sup>-2</sup> were used. Using a discrete dislocation dynamics method, creep of such crystals, in a case when the deformation geometry causes to primary formation of dislocations on a crystal surface, is modeled. Then lines of the majority of formed dislocations will be parallel, and will pass through all specimens. Therefore the modeling essentially becomes simpler, and the system becomes quasi-2D. Interaction of dislocations with each other and with surfaces of a specimen was taken into account by the model. It was supposed that dislocation formation occurs only on a surface of specimen. The uniaxial compression (along the greater side of a specimen), 3- and 4- point bend are modeled. The uniaxial compression case has the best accordance with experiment. Presumably it means that in this case dislocations which lines perpendicular to considered dislocations really are not formed.

P.S.B.37.

### STRUCTURE AND PROPERTIES OF ZIRCONIUM TUNGSTATE

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The structure and properties of zirconium tungstate was studied. A  $ZrW_2O_8$  ceramic was synthesized from  $ZrO_2$  and  $WO_3$  powders with the stoichiometric ratio of 1: 2 and temperatures 1100 and 1200  $^{0}$ C. It has been shown that the powder  $ZrW_2O_8$  has a cubic symmetry with lattice parameter a=9,154 Å. Thermal expansion coefficient was measured at temperature below  $800^{~0}$ C and it was shown that this coefficient up to temperature  $550^{~0}$ C is negative. The effect of the thermal expansion coefficient on the mechanical properties of composites based on aluminum alloys was studied.

P.S.B.38.

### PHONON THERMAL CONDUCTIVITY OF GRAPHENE

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The study of graphene thermal conductivity is of great importance, as its anomalous thermal and electrical conductivities (the largest so far) provide very good perspectives for graphene-based nanoelectronic devices. Thermal conductivity of graphene is basically phonon-based, since its electronic-based thermal conductivity represents less than 1 % of the total thermal conductivity at room temperature. To investigate thermal conductivity of graphene the Boltzmann equation in the approximation of relaxation time is hereby used. Relaxation time is determined, with three mechanisms of phonon scattering accounted simultaneously: at defects, at borders, and on phonons. Temperature dependence of thermal conductivity is determined numerically in the range of  $15-400~\rm K$ . The results obtained are in accordance with experimentally observed.

P.S.B.39.

## OPTICAL SPECIFICITY OF TWOLAYERED MOLECULAR NANOFILMS

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The changes of optical properties under boundary presence in thinnest molecular crystal nanofilm were theoretically investigated in this work. The dispersion law and possible states of excitons as well as their space distribution along boundary direction have been determined using adjusted Green's function method and also by combined analytical and numerical calculations. On the basis of real and imaginary part of relative permittivity, both absorption and refraction indices were determined, and the influences of boundary parameters on occurrence of a very selective and strictly discrete absorption were analyzed.

P.S.B.40.

### SYNTHESIS OF FERRITE CORE/SILICA SHELL NANOPARTICLES

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Presently oxide magnetic nanomaterials are considered to be of extreme significance to the society, because of wide range of potential applications in the field of biomedicine and bioengineering. Still, most of these applications require the magnetic particles to be coated with nonmagnetic and biologically compatible substance. For this purpose, silica has been widely used due to its biocompatibility, stability against degradation and possibility of modification with a wide range of functional groups. In this work, a possible approach for the coating of magnetite and ferrite nanoparticles with shells of amorphous silica has been presented. Nanoparticles of magnetite (Fe $_3$ O $_4$ ) and nickel ferrite (NiFe $_2$ O $_4$ ) have been synthesized by coprecipitation route using stable iron and nickel salts with sodium hydroxide as the precipitating agent and citric acid as the surfactant. Silica (SiO $_2$ ) shell was obtained by sol-gel process using tetraetylortosilicate (TEOS) as the precursor, directly in ethanol. The influence of reaction parameters (reaction time, core stabilisation procedure, etc.) on particle morphology, size and size distribution, has been investigated. Obtained core particles, as well as core-shell structures were characterised with electron microscopy (TEM, SEM) infra-red spectroscopy (FTIR) and X-ray diffraction (XRD).

P.S.B.41.

# THE INFLUENCE OF THE MICROSTRUCTURE ON THE DOMAIN STRUCTURE AND MAGNETIC PROPERTIES OF Nd-Fe-Al ALLOYS

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The present study investigated an alloy Nd<sub>60</sub>Fe<sub>30</sub>Al<sub>10</sub>(at. %) in the form of cylindrical rods with the diameters ranging from 1mm to 6mm. The rods were obtained by casting the material in a copper die. The casting temperature was 1370K. In all cases the material obtained consisted of crystalline and amorphous phases in proportions dependent on the rod diameter. Differences in the structure were also found in the axial cross section of the rods. This manifested itself as variations of the magnetic properties with distance from the axis (e.g. for a 6mm rod the coercivity for the regions located at the axis and close to the outer surface was 60 and 140 kA/m respectively. The investigation of the averaged phase structure using the X ray diffraction method revealed the presence of the pure Nd and Fe<sub>a</sub> as well as complex phases NdFeAl (Nd<sub>6</sub>Fe<sub>9.5</sub>Al<sub>4.5</sub>, Nd<sub>6</sub>Fe<sub>12.6</sub>Al<sub>3.8</sub>). Detailed investigation using high-resolution electron microscopy showed the presence of elongated grains of a two-component phase Nd<sub>5</sub>Fe<sub>17</sub> with dimensions of about 20x70 nm, as well as very fine crystalline precipitations with complex phase composition and a small quantity of the amorphous phase. Analysis of the polar cross section for these alloys revealed crystallographic orientation of large grains, which did not influence anisotropy of their magnetic properties. The investigation of the magnetic structure showed the presence of strong magnetic domains with sizes approaching 2 µm aligned with the rod axis and much smaller domains not exceeding 500nm without any specific orientation. The magnetic properties were studied using the magnetometric method. The microstructure of alloys was investigated using high-resolution electron microscopy (HR TEM) supplemented by the investigation of their chemical composition using X-ray spectrometry (EDX). The domain structure was studied using the method of magnetic force imaging (MFM).

P.S.B.42.

### POROUS ALUMINA SINTERED FROM DIFFERENT GRAIN SIZE POWDERS

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The microstructure of alumina ceramics based on powders with a different grain size has been investigated. An increase of nano-  $Al_2O_3$  powder content in the mixtures was found to change the pore structure of the corundum ceramics from a high-porosity ceramic skeleton with a well-developed system of channel-forming pores to ceramics with isolated pores. The change in the pore structure was observed for 50% porosity and caused an increase in the level of crystal lattice microdistortions. An increase in the sintering temperature from 1200 to 1650° C is shown to be responsible for a two-fold increase in the average crystallite size and for annealing of lattice defects at grain boundaries.

P.S.B.43.

# COROSION STUDIES OF NiMnGa SHAPE MEMORY ALLOYS IN VARIOUS COROSIVE ENVIRONMENTS

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Corrosion processes in metals substantially deteriorate their physico-chemical properties. The corrosive behaviour was studied in magnetic shape memory NiMnGa alloys. The process was investigated using voltamperometric method. Pure nickel was used as reference material. The measurements of open circuit potential (OCP) were applied for recording the dependence of current density I (A/cm²) on the potential E (V), in the range of applied potential -150 mV to 1500 mV, at the potential velocity change of 1 mV/s. The measurements were carried out at room temperature, using solutions of NaCl, NaOH and  $\rm H_2SO_4$ , respectively. It was found that the corrosion behaviour of NiMnGa alloys depends on the pH of the solution applied. The NiMnGa are more susceptible for corrosion than the pure nickel.

P.S.B.44.

# MECHANOCHEMICAL SYNTHESIS OF Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub>

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Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub> was prepared from the starting materials BaCO<sub>3</sub>, SrCO<sub>3</sub> and TiO<sub>2</sub> through solid state reaction. Mixtures of these oxides were mechanically activated using a high-energy ball mill at different time intervals from 0 to 120 minutes. X-ray diffraction was employed in order to determine the crystal structure and gave information about composition of phase variation. It was observed that after 40 minutes early synthesis of Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub> phase occurred. Particle size distribution along with scanning electron microscopy gave very useful information about powder morphology.

P.S.B.45.

### ANTIOXIDATIVE CAPACITY OF COMMERCIAL BEERS FROM SERBIA

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The purpose of the present work is to determine the antioxidant capacity (AC) of 5 commercial beers (Efes Draft, Calsberg, Pils Plus, Efes Pilsner, Staropramen) in Serbia markets. The AC indicates the degree of protection of a certain organism against oxidative damage provoked by reactive oxygen and nitrogen species. Also, investigation of AC would be helpful to better understand the beer flavour stability. Antioxidant activity was analysed using DPPH radical scavenging and ABTS radical cation scavenging activity. The Trolox calibration curves were plotted as a function of the percentage of DPPH radical scavenging activity and of the percentage of ABTS radical cation scavenging activity. The final results were expressed as milimoles of Trolox equivalents (TE) per liter of beer (mmol TE/L). All beers showed antioxidant power. The results of investigation are given in table.

Table: Antioxidative capacity of 5 commercial beers

Sample	Total antioxidant capacity mmol TE/L	
	DPPH radical scavenging activity	ABTS radical cation
		scavenging activity
$\mathbf{B}_1$	$0.60 \pm 0.01$	$0.21\pm 0.01$
$\mathrm{B}_2$	$0.50 \pm 0.02$	$0.24 \pm 0.02$
$\mathbf{B}_3$	$0.42 \pm 0.02$	$0.19 \pm 0.01$
${f B}_4$	$0.38 \pm 0.02$	$0.14 \pm 0.01$
$B_5$	$0.60 \pm 0.01$	$0.23 \pm 0.01$

P.S.B.46.

# CHARACTERIZATION SOLID, VISCOELASTIC AND LIQUID MATERIALS BY OPTO-MAGNETIC SPECTROSCOPY

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Optomagnetni fingerprint (OMF) is a new method of surface material investigation, which is based on light-matter interaction. Valence electrons and their electrical and magnetic forces are starting point of departure. Light-matter interaction will be different depending of covalent bonds, ion-ion, ion-dipol, dipol-dipol interacions presence in material surface (thin layer).

In order to investigate different types of materials we have investigated the solid materials (metal), viscoelastic matter (skin) and liquid (water). For each sample we took 300 digital images under the influence of white light and the white light under the Brewster angle. Using spectral convolution algorithm we made intensity-wavelength difference diagrams. Analyzing them it has been shown that average value (AV) and standard deviation (SD) are different for those three material types'. AV and SD are more compact for metal, water and skin, respectively.

P.S.B.47.

# RIETVELD REFINEMENT OF BARIUM TITANATE STANNATE CRYSTAL STRUCTURE

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The barium titanates have wide application in electronic industry as a dielectric and ferroelectric materials. The  $BaTiO_3$  doped with Sn is important for practical application in ceramic capacitors as well as in functionally graded materials. It is known that  $BaTiO_3$  materials have the typical perovsikite crystal structural. Their ideal crystal structure is a centrosimetric

cubic structure with Pm3m space group. However, the changes in temperature, pressure, and composition lead to phase transitions and crystal structure transformations.

In this study using by Rietveld refinement, we resolved crystal structure of barium titanate stannate (BTS)  $BaTi_{1-x}Sn_xO_3$  (x=0,0.025,0.05,0.07,0.10,0.12,0.15 and 0.20) solid solutions. The powders were prepared by simple solid state reaction at 1420 °C, in air for 2 hours. The structural investigations of the BTS samples were done at room temperature using an X-ray diffraction, Raman spectroscopy and TEM micrograph. The Rietveld refinement of the X-ray diffraction data was used to analyze the structural changes depending on amount of the Sn<sup>4+</sup> ions in the BTS. Obtained data show that increasing of Sn amount in the structure provokes the transformation of crystal structure from tetragonal to cubic one. We suppose that the absence of orthorhombic and rhombohedral phases is probably a consequence of phase (0.025 $\leq$ x<0.20) stabilization caused by method of sample preparation (high temperature solid state reaction).

P.S.B.48.

# DETERMINATION OF THERMAL CONDUCTIVITY OF THE INSULATION MATERIALS USING NUMERICAL CALCULATION OF THE PRESSURE INCREASE

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In the paper is presented the possibility of determination thermal conductivity for the insulation materials, which are used in the tanks for liquid carbon dioxide, in situ. For this purpose, was developed the mathematical model for description of the pressure changes in function of the ambient conditions and storage time. The application software was developed also for computation of the pressure increase two-phase mixture in tank, relating to the time, and the thermal conductivity determination of the insulating material. Verification of the program was done in function of exploitation incoming data. The numerical simulations of the pressure increase are done for various degrease of tank compliance. The influence of the ambient conditions is expressed by the heat transfer fluid in tank and the environment. Used incoming data are the temperature profile and sun heat flux characteristic for Serbia, in summer time.

P.S.B.49.

# CHARACTERIZATION OF DIVERSE BIO-COMPOSITE MATERIALS BY INDENTATION, SIMULATION AND INVERSE ANALYSIS

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Knowing the mechanical properties of bio-composite materials is very important especially when it is used as load carrying element as substitute for natural bone. For instance, properties of thermoplastic polymers (such as PLLA), usually used as matrix in bio-composites, in its solid state are strongly affected by processing conditions (i.e. temperature, pressure, etc.). This circumstance suggests that, the mechanical properties should be assessed after the processing is finished. This paper presents some preliminary results of a novel approach that uses in situ nanoindentation experiment for the purposes of material characterization. In the approach adopted here, the experiment is performed in order to collect data in the form of so-called indentation curve, namely the curve that correlates applied force during the experiment with achieved penetration into the material specimen. The same experiment is further simulated by the use of finite element method, where appropriate material constitutive model is adopted. In such way, simulated response becomes a function of the unknown material properties. The discrepancy function is then formed which quantifies the difference between measured and computed response. This function represents an objective function to be minimized in a subsequent step of the proposed strategy, by the use of appropriate non-linear mathematical programming algorithm. With the adopted approach it is possible to perform characterization of mechanical properties in more accurate way with respect to, for example traditional methods based on semiempirical formulae (e.g. Oliver and Pharr formula). The accuracy of assessed parameters can be a posteriori verified by the finite element simulation of the experiments on different scales.

P.S.B.50.

# KINETICS MODEL OF OXIDATIVE PROCESS IN BASIL-BASED SPREADS BY COLOUR ANALYSIS

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Basil-based spread, similar to traditional Italian, non heat-processed "pesto" sauce, which is limited to the very short shelf life due to oxidative procesess and its microbial load, was chosen to test the antioxidative properties of lactoferrin, metal-chelating protein, isolated from milk, which is an antimicrobial agent of broad spectrum. Enzymatic and non-enzymatic browning of basil-based pesto spreads was monitored using colour changes, by means of multivariate colour image analysis. The objective of the study was to assess the antioxidative potential of lactoferrin in combinations of organic acids (ascorbic, citric, lactic) and NaCl on browning and prolonged lipid oxidation in fresh basil-based emulsions.

The process of colour changing, occuring due to oxidation processes of row vegetable or fruit-based foods, known as "browning", can be observed by an evaluation algorithm describing the colour coordinates changes in digitalised images. The common practice in the assessment of food colour is to use spectrophotometers or light sensitive cells to quantify colour characteristics. The most frequent instruments evaluate only restricted areas of food samples or overall light reflectance from the entire surface of the food matrix, thus being not appropriate for inhomogenous food products, such as basil-based spreads. The coloured images were taken with a common, digital CCD camera, while basic colour informations of recorded digitalized images, were expressed in *R*, *G*, *B* colour coordinates, during oxidation of samples, and afterwards transformed to frequency colour distribution of colour mentioned coordinate values. Colour image analysis is an effective methodology, able to measure average chromatic parameters of non-homogenous surfaces.

It was shown that different concentrations of ascorbic acid (0.5 g·kg<sup>-1</sup> and 1g·kg<sup>-1</sup>) had main influence on browning reactions according to obtained kinetic constants of browning (a, n,  $y_0$ ,  $k_0$ ,  $k_1$ ), while lactoferrin presence had impact on prolonged lipid oxidative stability.

Key words: colour coordinates, kinetics, food, oxidation, browning.

P.S.B.51.

# THE INCREASE OF REACTIVITY OF THE COPPER-NICKEL SULFIDE ALLOY BY TEMPERING

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The tempered alloys of the nickel and copper sulfides were prepared by water jet atomizing. The researches of the influence a solidification rate on the reactivity of the granulated alloys were carried out by electron microprobe analysis, high-temperature X-ray diffraction and differential scanning calorimetry. Feature of the tempered samples is finely dispersed microstructure formed from the metastable phase Ni<sub>3 + x</sub>S<sub>2</sub> and Cu<sub>2-x</sub>S. The calculation of unit cell parameters and thermal expansion factors indicates the anisotropy of thermal deformation and growth of disorder into the crystal lattices of nickel and copper sulfides in tempered alloy. It is shown experimentally that the dissolubility of the alloy granules in the autoclave and electrochemical processes increases more than twice.

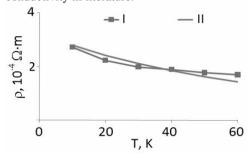
This work was supported by the Ministry of Education and Science of the Russian Federation (State contract  $N_0$  02.740.11.0821).

P.S.C.1.

## LOW-TEMPERATURE ELECTRON TRANSPORT PROPERTIES OF CARBON NANOTUBES

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The low-temperature peculiarities of electron transport properties of carbon nanotubes may be described using the classical Drude, Wiedemann-Franz and Mott formulas. In our case the electron relaxation time is calculated by the quantum mechanical techniques [1], taking into account multiple elastic scattering of electrons by impurities and structural irregularities that are formed in nanotubes during their synthesis [2]. The results of our calculations showed that the low-temperature behavior of the electrical conductivity, thermal conductivity and thermopower in CNTs is determined by elastic electron scattering on short range ordered regions. Moreover, for the resistance and thermal conductivity (e.g. Fig.1 and 2) the magnitude of carrier concentration is determinant but for thermopower the carrier concentration is not important. This may be a reason of a large dispersion of data on electrical resistivity and thermal conductivity in literature.



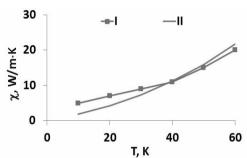


Fig. 1 Curve I – temperature dependence of resistivity for thin films of CNTs with a thickness of 0.5 microns to 10 microns (the diameter of a nanotube 10 nm) [3] and curve II corresponds to the calculated resistivity at n  $\sim 10^{23}$  m<sup>-3</sup>.

Fig. 2 Curve I – the thermal conductivity of the sample similar to the tissue SWNTs, measured along the tube axis [4] and II corresponds to the electron thermal conductivity calculated for n  $\sim 3\cdot 10^{27} \text{ m}^{-3}$ .

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P.S.C.2.

# MAGNETIC CRYSTALLITES ENCLOSED IN CARBON MATRIX FOR PROSPECTIVE BIOMEDICAL APPLICATION

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The materials obtained are in a form of composite beads built of magnetic nanocrystallites (Fe<sub>3</sub>C, Ni, Co) dispersed in a bioinert matrix. The as-obtained beads have relatively broad size distribution, ranging from few up to 200 microns. Thus, further reduction of the beads, down to four microns, by ball milling was implemented. Good magnetic properties of the beads, especially high saturation magnetization, make them suitable for applications as magnetic carriers in targeting drug delivery or bioseparation. The matrix is build of two form of carbon, i.e. amorphous carbon and graphite. The matrix provides stabilization of the metallic crystallites and renders the possibility of surface functionalization.

P.S.C.3.

# MULTIPLE SPIN DYNAMICS IN Co<sub>1+y</sub>Al<sub>2-y</sub>O<sub>4</sub> SPINEL DILUTED IN AMORPHOUS SiO<sub>2</sub>

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We report observation of multiple spin dynamics in nanocrystalline  $Co_{1+y}Al_{2-y}O_4$  spinels. The  $Co_{1+y}Al_{2-y}O_4$  nanoparticles dispersed in an amorphous  $SiO_2$  matrix were synthesized by the sol-gel technique. The dynamic (ac) magnetic susceptibility measurements are sensitive tool to detect phase changes at low-temperature. The measurements of temperature dependence of the ac magnetic susceptibility reveal multi peak spectra. Positions of the peaks show marked temperature dependence.

P.S.C.4.

# ACCELERATED POLYMORPHOUS TRANSFORMATION OF ALUMINA IMPED COPPER ALUMINATE SPINEL FORMATION

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Thanks to its high melting point, good chemical stability and mechanical strength, spineltype solids MAl<sub>2</sub>O<sub>4</sub> (M<sup>2+</sup>-metal) are widely used as catalysts or catalyst supports. In environmental catalysis magnesium aluminate spinel, (MgAl<sub>2</sub>O<sub>4</sub>) can be used as catalyst for SO<sub>x</sub> abatement, while copper aluminate spinel, (CuAl<sub>2</sub>O<sub>4</sub>) plays an important role in NO<sub>x</sub> reduction to N<sub>2</sub>, as well as in oxidation of CO. Zinc aluminate spinel, (ZnAl<sub>2</sub>O<sub>4</sub>) in combination with copper is used as low pressure methanol synthesis catalyst, or as low temperature shift catalyst. The only industrial process (Esterfip-H) which applies heterogeneous catalyst for biodiesel synthesis uses a zinc aluminate spinel catalyst. In our previous paper the reaction constants of ZnAl<sub>2</sub>O<sub>4</sub>, MgAl<sub>2</sub>O<sub>4</sub> and CuAl<sub>2</sub>O<sub>4</sub> formation were determined. These reactions occur between metal oxide and alumina support at higher temperatures. The rates of spinel formation decrease in the sequence ZnAl<sub>2</sub>O<sub>4</sub> > MgAl<sub>2</sub>O<sub>4</sub> > CuAl<sub>2</sub>O<sub>4</sub>, irrespective of precursor of the alumina support used. Simultaneously with spinel formation sintering process occurs, usually as undesirable side effects. Spinels of ZnAl<sub>2</sub>O<sub>4</sub>, MgAl<sub>2</sub>O<sub>4</sub> and CuAl<sub>2</sub>O<sub>4</sub> were synthesized by impregnation of alumina, or their precursors, (gibbsite, boehmite, and γ-Al<sub>2</sub>O<sub>3</sub>, fraction below 63 μm, all synthesized in our Laboratory) with corresponding metal salts,  $Zn(NO_3)_2 \cdot 6H_2O_1$ Mg(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, and Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O in water solution. Equal molar ratios of two valent metal salts and alumina were used in order to guaranty the conditions for spinel formation. The impregnated sample precursors were dried at 105°C overnight, calcined at 350°C for 4 hours in air, following thermal treatment at 800-1100°C for 1,3,5,7 and 10 hours in air. Specific surface area, (S) measured by LTNA, was taken as indicator of sintering, while SEM and AES analysis were used for morphology and metal distribution investigation. In samples with zinc and magnesium ions, decelerated polymorphous transformations of alumina occur, compared to pure aluminum compounds. The impeded phase transformation of alumina coincides with decreased degree of sintering, defined as  $[\alpha_s = (S_o - S_l)/S_o]$ . Copper ions accelerate polymorphous transformations of alumina, and consequently the CuAl<sub>2</sub>O<sub>4</sub> spinel formation is slower. Accelerated sintering, which is proved by strong decrease of surface area, could be explained by accelerated phase transformations of alumina support. Copper ions d<sup>9</sup>(Cu<sup>2+</sup>) can cause distortion of local ligand symmetry of transient forms of alumina, which on macroscopic level is manifested as its polymorphic transformation (Jahn-Teller effect). It seems that accelerated polymorphic transformation of alumina caused by copper ions, slowing the creation of CuAl<sub>2</sub>O<sub>4</sub> spinel.

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P.S.C.5.

# TRANSFOMATIONS AND MICROMECHANICAL INSTABILITY BEHAVIOR OF POROUS CERAMIC

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It has been studied the mechanical behavior under compression test zirconia ceramics. It was found a micromechanical instability of rod-like structures formed after sintering of nanopowders and it was shown a high micro quasi-elastic deformation this material up to 2% without fracture.

P.S.C.6.

# THE ANALYSIS OF STABILITY OF THE ELECTROSPINNING PROCESS OF FORMING PVB-SiO<sub>2</sub> NANOCOMPOSITE FIBERS

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The PVB-SiO<sub>2</sub> composite nanofibers were obtained by the electrospinning process. The experiments were carried out with PVB solution in concentration of 10 wt% where as the solvent was used ethanol. The silica nanoparticles were added in the solution in different content of 1, 3 and 5 wt% SiO<sub>2</sub>, and they were both modified and unmodified with amino-silane. The impact of the parameters of the electrospinning process on the produced PVB-SiO<sub>2</sub> nanocomposite fibers was tested. The structures of the PVB-SiO<sub>2</sub> nanocomposite fibers were investigated using scanning electron microscopy (SEM) and characterized by Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC) and thermogravimetric (TG) analysis. The morphology and distribution of the resulting nanofibers were analyzed using software Image - Pro Plus.

P.S.C.7.

# PREPARATION, CHARACTERIZATION AND UP-CONVERSION OF $\mathrm{Er^{3+}}$ DOPED YTTRIUM-LUTETIUM OXIDE NANOPHOSPHOR

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In this report we demonstrate visible up-conversion emission of erbium doped yttrium-lutetium ( $(Y_{0.5}Lu_{0.5})_2O_3$ ) oxide nanophosphor and discuss mechanisms responsible for pumping the  $Er^{3+}$  upper levels. For the material production we explored synthesis route based on the polymer complex solution method. In this type of synthesis polyethylene glycol is used both as fuel for the combustion reaction, and as nucleation agent for the crystallization process. Detailed information on nanopowder phase, morphology and crystallinity were obtained using X-ray diffraction and transmission electron microscopy (TEM) measurements. X-ray diffraction analysis showed that presented synthesis procedure yields pure-phase, well crystallized nanopowder with the particle dimensions in the 30-50nm range, as observed from TEM images. Up-conversion is characterized by intense red emission under near infrared excitation by optical parametric oscillator. Emission kinetics (i.e. emission decay) are recorded and presented.

P.S.C.8.

# MONODISPERSE LUMINESCENT PARTICLES OF Y<sub>2x</sub>Gd<sub>x</sub>O<sub>3</sub>:Eu SOLID SOLUTIONS

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One of the most important applications of monodisperse particles is luminescent coatings and highly efficient light sources. The most promising luminescent materials for such applications, namely rare-earth oxides and oxisulfides, at the same time require the largest amounts of energy during synthesis. Therefore, development of energy-saving methods of synthesis of monodisperse particles of rare-earth oxides with improved luminescent properties is very vital task. Microwave treatment possesses many advantages in comparison with conventional heating methods, including higher velocity of heating, homogeneity of heat distribution and lower power inputs. Earlier we've developed method of microwave-assisted synthesis of monodisperse RE-doped yttria powders consisting of spherical particles and possessing strong luminescence. Comparing to conventional methods of synthesis microwaveassisted process allows increasing the yield of reaction dramatically. In present work we've developed new method of microwave-assisted synthesis of Y<sub>2-x</sub>Gd<sub>x</sub>O<sub>3</sub>:Eu solid solutions performed a study of influence of Y:Gd ratio on morphology and luminescent properties of monodisperse oxide particles. We've established linear dependency of mean size of particles on Y:Gd ratio. On the other hand dependency of intensity of luminescence on Y:Gd ratio has a clear maximum. The work was supported by RFBR (grants # 09-03-01067 and 10-02-91167-GFEN a) and grant of President of Russian Federation for support of young scientists (MK-2607.2011.3).

P.S.C.9.

# SYNTHESIS AND CHARACTERIZATION OF NANOSTRUCTURED BOEHMITE POWDERS FOR OBTAINING TRANSITION GAMMA ALUMINA

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Among the transition aluminas,  $\gamma$ -alumina is one of the most important oxides, attracting much attention for years because of its potential for broad application in advanced catalysts, adsorbents, composite materials, membranes etc. Recently, nanostructured y-alumina with structural and morphological specificity such as high surface area, porosity, and chemical activity has attracted enormous interest from both fundamental and practical viewpoints. Boehmite (γ-AlOOH) is an important inorganic precursor for obtaining γ-Al<sub>2</sub>O<sub>3</sub>. When it is heated, boehmite undergoes a topotactic transformation into gamma phase. A crucial issue that demands much more research is better understanding of the effects of processing parameters, boehmite structure and further heat treatment conditions on the final structure of gamma phase. In this work, the sodium-aluminates solutions from Bayer liquor have been used as raw materials for boehmite preparation. The research has been focused on elucidating the influence of process variables during the neutralization of aluminate solutions with sulfuric acid (solution concentration, pH, temperature, non-surfactant agent) on the structural and morphological characteristics of boehmite. Boehmite phase was obtained without additive only from solution that had a concentration of [NaOH] = 2.46 M, [Al(III)] = 1.56 M. Addition of glucose as a nonsurfactant agent to the starting aluminate solution leads to the formation of nanocrystalline boehmite with estimated average crystallite size less than 3 nm and high surface area (over 300 m<sup>2</sup>/g). Addition of non-surfactant agent to the sodium aluminate solutions affects interparticles forces which led to the formation of spherical boehmite particles in all solutions. During heating at 500°C, the boehmite nanostructures undergo an isomorphous transformation to nanostructure  $\gamma$ -alumina, which can retain the morphology of the parent boehmite nanostructures.

P.S.C.10.

# NANOCRYSTALLIZATION OF GLASS IN THE SYSTEM LI<sub>2</sub>O·GEO<sub>2</sub>·P<sub>2</sub>O<sub>5</sub>

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The glasses from  $\text{Li}_2\text{O}\cdot\text{GeO}_2\cdot\text{P}_2\text{O}_5$  system are very interesting as potential solid electrolytes. For practical use, it is necessary that the conductors possess good chemical stability and to be easily manufactured. One of the routes for synthesis of such materials is the crystallization of these glasses. This method requires the knowledge of crystallization behavior of the selected glass. The glass  $22.5\text{Li}_2\text{O}\cdot10\text{Al}_2\text{O}_3\cdot30\text{GeO}_2\cdot37.5\text{P}_2\text{O}_5$  [mol%] was used for investigation. In this composition  $\text{Ge}^{4+}$  was partially substituted with  $\text{Al}^{3+}$ . The glass was melted in platinum crucible at T=1400 °C during t=30 min. The glass transition temperature  $T_g$ =518°C, the crystallization peak temperatures  $T_{pl}$ =665°C,  $T_{p2}$ =736°C and the liquidus temperature  $T_i$ =1074°C, were determined. The crystallization experiments were performed under isothermal conditions by heating a glass at 660-800 °C for t = 1-100 h. and one stage regime of heating was employed. XRD analysis showed that this glass crystallized by the primary crystallization. As primary  $\text{LiGe}_2(\text{PO}_4)_3$  phase is formed, while  $\text{GeO}_2$  appeared as the secondary one in quantitative amount < 0.05. The volume crystallization mechanism of these crystalline phases was detected. The size of crystals was in the range of 50-200 nm.

P.S.C.11.

# OPTICAL PROPERTIES OF NANOCOMPOSITE FILMS BASED ON Ag/PMMA SYSTEM

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As continue of our previous studies, three silver organosols with different nanoparticles sizes were used to obtain nanocomposite films based on Ag/PMMA system. Among polymeric materials, PMMA is well known as a polymeric glass and engineering plastic with a wide range of applications. One of the objectives of this work is to gain better insight into the properties of this material upon incorporation of small amount of silver nanoparticles. Silver nanoparticles were synthesized in various organic solvents (toluene, 1.2- dichlorobenzene ) in order to obtain different sizes of nanoparticles: 7.2 ±2.8 nm, 13.7±2.7 nm and 22.7±3.5 nm. By varying the heating temperature, solvent and reaction time, we could control the size of nanoparticles. In the second step, nanocomposites Ag/PMMA were prepared by in-situ bulk polymerization of methyl methacrylate in the presence of appropriate amount of silver nanoparticles. The size distribution and morphology of the silver nanopaticles in the nanocomposite films were determined using TEM measurements. The influence of size and dielectric property of surrounding media on surface plasmon absorption band of silver nanoparticles are discussed. UV-vis and FTIR spectroscopy have been applied to support the change in the optical and chemical properties of the silver organosols, as well as transparent and coloured Ag/PMMA nanocomposite films.

### P.S.C.12.

# RHEOLOGICAL CHARACTERIZATION OF MAGNETORHEOLOGICAL FLUIDS WITH BIMODAL IRON PARTICLES

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Rheological properties of magnetorheological fluids (MRF's) with carbonyl iron powders based on synthetic oil are presented. Two types of carbonyl iron powders with average particle size of 1µm and 5µm respectively were used for synthesis of bimodal MRF's. As a stabilizer the hydrophilic nanosilica was used. Two fluids, with various proportions of the respective carbonyl iron powders, were used to study the influence of composition on the rheological properties of the MRF's. The application of bimodal powders without stabilizer resulted in enhanced magnetorheological effect. The rheological data shows that the viscosity of the synthesized MRF's, measured at a shear rate of 0.1 1/s, for a magnetic field of 0.2 T, increased by three order of magnitude, when compared with the value without magnetic field.

P.S.C.13.

# SHEAR THICKENING FLUIDS BASED ON NANOSIZED SILICA SUSPENSIONS FOR ADVANCED BODY ARMOUR

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The shear thickening fluid (STF) – para-aramide composites are developed in the light of their potential application in the smart body armour. The study reports on the rheological behaviour of the nanosized silica suspensions. Depending on the oligomer chemical structure and molecular weight we observe different behaviour under the shear stress. The addition of the colloidal shear thickening fluids, to para-aramide woven fabrics (Twaron® CT709) showed slightly enhanced ballistic penetration resistance of the elaborated system.

P.S.C.14.

# CHARACTERIZATION OF NANOSTRUCTURED POLYURETHANE ELASTOMERS VIA ATOMIC FORCE MICROSCOPY

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Atomic force microscopy (AFM) is a very powerful method of the characterization of complex polymer systems. This contribution will summarize our AFM results made on polycarbonate-based polyurethane (PC-PU) elastomers prepared from aliphatic polycarbonate (PC) diols of MW either 1000 or 2000, hexamethylene diisocyanate and 1,4-butanediol. Some PC-PUs also contained layered nanoadditives (Bentonite for organic systems and organically modified montmorillonite). Fracture areas of PC-PU sheets (after previous freeze-fracturing at the temperature of liquid nitrogen) and surfaces of films were measured. All PC-PUs are flat with the roughness on the nm scale. The topography and also the phase images (i.e., homogeneity of broken-area surfaces) depend significantly on the contents of individual components (especially on the polycarbonate diol amount; the higher PC diol content, the smoother broken-area surface) and on the presence/absence of nanofillers, which are, i.a., well visualized in both types (film, sheet) of surface images.

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P.S.C.15.

# MODIFIED THERMOPLASTIC IMPREGNATED MULTIAXIAL ARAMID FABRICS WITH NANOSILICA REINFORCEMENT

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A report of manufacture of new fabric forms from hybrid laminated multiaxial composites with enhanced thermo mechanical properties is presented. Thermal and dynamic mechanical analyses of fabricated hybrid composites were employed in order to analyze the optimal processing conditions and reinforcement contents. Dynamic mechanical analysis shows that introduction of 5 wt% silica nanoparticles in the composite of polyurethane-aramid-poly (vinyl butyral) leads to significant improvement in mechanical properties, and the addition of silane coupling agents yielded maximal values of storage modulus for hybrid nanocomposites. The introduction of silane adhesion promotors and fixative cross-linker (glutaraldehyde) increased the bonding between particles through silane and induced a linkage with the amide groups present in the aramid fabric and OH groups from poly (vinyl butyral). Promoted bonding and nanoparticle dispersion reduced the mobility of macromolecules, which is shown by the decrease of damping factor for the polyurethane-aramid-poly (vinyl butyral) composite. The increase of glass transition temperature of composites with amino functionalized silica nanoparticles showed their contribution to the materials improved thermal stability.

P.S.C.16.

# MECHANOCHEMICAL SYNTHESIS AND CHARACTERISATION OF NANOCRYSTALLINE BISMUTH SELENIDES (BiSe, Bi<sub>2</sub>Se<sub>3</sub>)

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Mechanochemical synthesis of bismuth selenides (BiSe, Bi<sub>2</sub>Se<sub>3</sub>) was performed by highenergy milling of bismuth and selenium powders in a planetary ball mill. The particle size distribution and the specific surface area of Bi/Se and 2Bi/3Se powder mixtures were analysed at increasing milling time. The products were characterised by X-ray diffraction (XRD), differential scanning calorimetry (DSC) and transmission electron microscopy (TEM). The presence of bismuth selenide phases was observed after only 1 min of milling and full conversion into hexagonal BiSe phase (nevskite) and rhombohedral Bi<sub>2</sub>Se<sub>3</sub> phase (paraguanajuatite) was reached after 10 min of milling. The nanocrystalline nature of both mechanochemically synthesised bismuth selenides was confirmed and their optical band gap energies were obtained on the basis of the recorded absorption spectra in UV-Vis spectral region.

P.S.C.17.

### MECHANICAL SYNTHESYS OF MAGNESIUM BASED NANOCOMPOSITES

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The solid state bonding of hydrogen in metals provides several advantages: the density of hydrogen is high, which is ideal for transportation, there is no risk of leakage or explosion, and finally, the hydrogen retained by this method has high purity, which is essential for its utilization in fuel cells. Among the metal hydrides, magnesium hydride has been considered as solution for energy storage since exhibits a high gravimetric density of hydrogen. Anyhow the slow sorption kinetics give rise to several problems that has to be solved before hydrogen enter to the economy. To solve this problem, two methods have been proposed: a decrease of crystallite size of magnesium to nanoscale size through high-energy ball milling and the use of suitable catalysts. We have investigated combined influence of both mechanical milling and addition of  $TiB_2$  and SiC additive to  $MgH_2$  on its desorption properties. Microstructural and morphological properties has been correlated to the desorption properties. The considerable improvement is desorption properties has been achieved.

P.S.C.18.

# LOW TEMPERATURE MECHANICAL CHARACTERISTICS OF TI Grade 2, PRODUCED BY DIFFERENT METHODS OF SEVERE PLASTIC DEFORMATION

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Physical and mechanical properties of the nanostructured materials can be improved by use of combined methods of the severe plastic deformation (SPD). In this work, with the help of various SPD methods (equal-channel angular pressing (ECAP), quasi-hydro extrusion (QHE), cryorolling (CR), and their combination) the eight different structural state of polycrystalline Ti Grade 2 were produced: 1) the initial coarse-grained Ti Grade 2, produced by hot forging; 2) the nanostructured state, produced by ECAP of initial Ti Grade 2 (8 passes of ECAP at 720 K); the states 3-7 produced by QHE of the state 1 at 300 or 77 K to 32-55 % of deformation; 8) - the state 2, subjected to CR at 77 K to 50 %. Values of microhardness H<sub>V</sub> were measured at 300 K, yield stress  $\sigma_{0.2}$  and deformation to failure  $\varepsilon_f$  were registered at temperatures 4.2 - 300 K under uniaxial compression of specimens with strain rate  $4.10^4 \, c^{-1}$ . Average grain sizes were established by transmission electron microscopy and changed from 20 µm to 0.1 µm for the different investigated structural states. The largest increase of  $H_V$  and  $\sigma_{0.2}$  values is registered for combined action of ECAP and QHE (the latest was made at 77 K to 53 % of deformation; the state 7). For example, at temperature 4.2 K under compression the  $\sigma_{0.2}$  values increase by 86 % in comparison with the  $\sigma_{0,2}$  of initial Ti Grade 2 and by 13 % against the  $\sigma_{0,2}$  of ECAP Ti Grade 2. It worth to note that plasticity of the nanostructured Ti Grade 2 in this high-strength state remains at level of 10-15 % in all temperature interval. Also, peculiarities of different nanostructured states, which influence on low temperature mechanical characteristics of Ti Grade 2, are discussed.

P.S.C.19.

# ON THE KINETICS OF REACTIONS TAKE PLACE DURING MECHANOCHEMICAL SYNTHESIS OF W-Cu AND Mo-Cu NANOCOMPOSITES FROM THE OXIDE COMPOUNDS

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In the present study, W-Cu and Mo-Cu nanocomposites were prepared separately by reactive milling of CuO and pure Mg along with WO<sub>3</sub> and MoO<sub>3</sub>, respectively. The structural evolutions of the powders at various stages of the processing were studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses. In both systems, in-situ reduction of the oxides and formation of W-Cu-MgO and Mo-Cu-MgO composites were verified by XRD. Furthermore, both processing reactions completed after about 16 min of milling. On the basis of thermodynamic properties of the reactants, XRD investigation, and temperature monitoring of the vial outside wall, the succession of the reactions take place during milling were studied. It was found that, in both systems, the reactions follow a kinetic path similar to the one associated with mechanically induced self-propagating reactions (MSR). It was also found that that the amount of heat generated from the CuO reduction is responsible for the accelerated rate of the second reaction.

P.S.D.1.

# REMOVAL OF PHARMACEUTICALLY ACTIVE COMPOUNDS BY MESOPOROUS ZSM-5 ZEOLITE

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Introduction of mesopore regions into initially micropore zeolite structures incresases the range of molecules zeolite can potentialy interact with, while presearving its active sites. In recent years, a novel route for mesopore formation via silicon extraction by hydroxides has been proposed. In this work zeolite ZSM-5, a material well known for its selective adsorbing and catalytic properties was modified by desilication for the purpose of removal of pharmaceutically active compounds (atenolol, diclofenac sodium, salicylic acid and bisphenol A) from aqueous solutions. The samples were fully characterized. The obtained ZSM-5 zeolite containing mesopore regions preserved its crystalline structure and acidity distribution upon modification. The adsorption capabilities of mesoporous ZSM-5 for removal of the selected pharmaceutically active molecules were compared to those of the parent, unmodified ZSM-5 zeolite.

P.S.D.2.

# THE ECO-FRIENDLY METHOD OF THE BIOACTIV COMPOUND EXTRACTION

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It is well known that biological active substances – terpens, alkaloids, proteins and other ones are situated in the plant cell. And to intensify the extraction process it is necessary to disrupt the cell wall. One of the methods of enhancement extraction process is the mechanical treatment of biomass materials with ultrasound. These methods allowed us to intensify the targets components extraction process. The main component of cell wall is cellulose. To improve extractives substances production cellulose degrading enzymes can be used. Combination of these methods: mechanical and biotechnological treatment of biomass under certain conditions can be allowed us to intensify the recovery process even more. It is important to develop new sustainable method of processing renewable biomass for chemicals production. Application of enzymes and ultrasonication of biomass allowed us to create eco-friendly technologies of these materials processing.

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P.S.D.3.

# NOVEL MECHANOCHEMICAL METHOD OF BIOPLASTICS MANUFACTORING FROM AGRICULTURE WASTES

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It is vital target for China to manufacture lignocellulose panel and bioplastics from agriculture wastes because of poor industrial wood. Composition of wood and cereal straw is enough similar besides ash amount brought about a large content of biogenous silica in row straw. Production of ecological friendly bioplastic without synthetic adhesive is discussed in present work. Impact of natural additives, mechanical treatment as well chemical treatments on mechanical properties of products was investigated. It was shown the mechanical behaviors of produced straw-based panel are not worse of those produced with phenolics binders.

P.S.D.4.

## IRRADIATION AGING OF CHLOROSULPHONATED POLYETHYLENE RUBBER BLENDS

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Two chlorosulphonated polyethylene rubber (CSM) blends with polychloroprene (CR) and acrylonitrile butadiene rubber (NBR), CSM/CR and CSM/NBR with different content of CR and NBR were used to prepare composites with a cure system based on sulfur. Rubber composites were prepared on a laboratory-size (300x600mm) two-roll mixing mill maintained at  $40\pm5^{\circ}$ C. Torque curves, measured with a moving die rheometer at a temperature of 433 K, were used to characterize the vulcanization process. To vary the cure level, samples of each compound were vulcanized at 433 K at different times, according to the information obtained from the rheometer data. The mechanical properties were performed using tensile tester machine (Zwick 1425) at room temperature. The samples were irradiated with gamma rays at ambient conditions with 100, 200 and 400 kGy. From swelling data, the diffusion coefficient of toluene in CSM/CR and CSM/NBR was evaluated, taking into account the influence of polymer structure and crosslink density. The gamma radiation resistance of composites was determined from the tensile strength and crosslinking densities after prolonged exposure to  $\gamma$ -irradiation (dose rate of 10 kGyh-1 and total absorbed dose of 100, 200, 300 and 400 kGy).

Keywords: CSM/CR and CSM/NBR rubber blends composites, irradiation, mechanical and swelling properties.

P.S.D.5.

## DIGITAL RADIOGRAPHY ON MONITORING OF CONCRETE PUMP MADE BY CARBOTECH COMPOSITE MATERIAL

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On truck-mounted concrete boom pump 1st, 2nd and 3rd sections are made of high strength steel and 4th, 5th and 6th boom sections are made of light and resistant cifa carbotech composite material. This second part of truck is under vibration, stress and strain so is important to monitoring which will be the carbotech composite material response. Digital radiography is non destructive testing on monitoring and diagnostic, during production and services life of product that is earning its place in the NDT market, as specialists realize this technology surpasses film. In this article will focus the digital radiography on carbotech composite materials, the energy, noise ratio, sensitivity, image quality, definitions of defects border. We used the scanner CRP50, plate PS. On the plate made from carbotech composite materials, thickness 5mm, 10mm and 15mm have done cylindrical holes with different diameter and depth. The results are very satisfactory.

P.S.D.6.

## ELECTRICAL PROPERTIES INVESTIGATION IN POLYSTYRÈNE/POLYANILINE COMPOSITES

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Reducing conduction threshold by the elaboration of new composite materials represents a technological interest since an excessive amount may affect other properties of the materials such as mechanical and optical properties. Conducting composites powders were chemically prepared by in situ polymerization and doping of aniline in presence of polystyrene, at room temperature. AC electrical properties measured in the frequency range of 10<sup>-1</sup> to 10<sup>7</sup> Hz are reported and the frequency behavior of electrical conductivity was investigated as a function of Polyaniline (PANI) concentration. The experimental conductivity was found to increase continuously with PANI content and is well explained by percolation theory, with a relatively low percolation threshold. These powders served to synthesize transparent antistatic films. As for powders, the films exhibited an enhanced electrical conductivity with increasing PANI content because of the percolation of PANI phase in the polystyrene matrix which was found at a higher value due to the destruction of the presumed core-shell structure by the used solvent. The structure of the films was investigated using Raman spectroscopy and X ray diffraction technique. Thermal properties were also studied by TGA and DSC measurements.

P.S.D.7.

#### HUMATE MATERIALS FOR SOIL REMEDIATION

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Ecologically friendly humate materials are produced via powder technology of humin containing raw, as peat or brown coal. Solid state reaction with alkali leads to the formation of humates having reactive "helate" groups. Diminishing of humate polyphenol molecules size, formation of phenol and chelate groups are investigated under different reaction conditions. Adsorption of humate thin layer on the surface of clay and silica soil particles results in formation of fertile soil. The humates molecules containing heteroatoms as nitrogen are adsorbed weaker than humate polymers without heteroatoms. Effect of powder products is checked for the benefication of soil in salted and desertificated regions of Kulunda, West Siberia. Pilot line with productivity up to 200 kg of powder product per hour is designed.

P.S.D.8.

#### SEROTONIN CONTAINING POWDER MATERIALS FROM PLANT RAW

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Serotonin or 5-hydroxytryptamine is a monoamine neurotransmitter, located in the gasrointestinal tract and in the central neurvos system of animals and humans. It is a well-known contributor to feelings of well-being; but now it is perspective not only for medicine applications but as the component of functional food, plant growth stimulator and flower concervant. Mechanochemically assisted solid state technology of serotonin production is developed from nonfruit parts (leaves, shoots and bark) of sea-buckthor (*Hippophae rhamnoides L.*). Powder materials with concentration near 2 mass% of serotonin was checked as the source of pure serotonin and as the fodder additives. Biological experiments with animal demonstrates the immuno stimulating activity, enhancing of moving activity in winter condition and stress defending properties of ecologically friendly powder preparation.

P.S.D.9.

#### HEAVY METAL CONTENT DETERMINATION IN DOMESTIC PEACHES

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Negative effect of pollution is widely recognised and consideration of heavy metal concentrations in food (vegetables, fruits) from different growing fields is necessary in order to help prevention of food contamination. The concentrations of heavy metals (Pb, Cd, Fe and Cu) in 6 different domestic peaches samples collected from 6 different locations in Nis (South Serbia region), were determined by inductively coupled plasma-optical emission spectrometry (ICP-OES). It is observed that metal concentrations in peaches samples go from 0,1040 to 0,0800 mg/kg of fresh fruit weight (f.w.) for Pb, 0,0005 and 0,0015 mg/kg f.w. for Cd, 5,170 and 9,970 mg/kg f.w. for Fe and 0,7520 and 1,1915 mg/kg f.w. for Cu. Therefore, heavy metal concentrations in peaches are in acceptable ranges according to World Health Organization (WHO).

P.S.D.10.

#### THERMOOXIDATIVE STABILITY OF NANOSILICA-BASED UREA-FORMALDEHYDE HYBRID COMPOSITE WITH 4-CHLORO-3-NITRO-2*H*-CHROMEN-2-ONE

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Interest in the development of new organic/inorganic nano-composites has grown in recent years due to a wide range of potential use of these materials. These hybrids constitute a class of advanced composite materials with unusual properties, which can be used in many fields such as optics, electronics, mechanics *etc.* Coumarins are used in the fields of biology, medicine, and polymer science. Coumarin polymers possessing antimicrobial activity have not received considerable attention in the literature. However the reported coumarin polymers possess variety of functions and appear to be interesting. Although there is a huge number of reports on monomeric coumarin derivatives, there are only a few reports on coumarin polymers. In this study, the thermooxidative stability of nanosilica-based UF hybrid composites (UF with SiO<sub>2</sub>-Resin 1 and UF + SiO<sub>2</sub> + 4-chloro-3-nitro-2*H*-chromen-2-one-Resin 2) with formaldehyde to urea (F/U) ratio (0.8) was investigated by thermo-gravimetric analysis (TG), differential thermal gravimetry (DTG), differential thermal analysis (DTA) and differential scanning calorimetry (DSC) supported by data from IR spectroscopy. The free formaldehyde percentage was determined for all samples.

P.S.E.1.

## SYNTHESIS, CHARACTERISATION AND BIOLOGICAL ACTIVITY OF A BIOLOGICALLY ACTIVE BRIDGED DIPHOSPHONIUM COMPOUND

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In the reaction of 2-(diphenylphosphino)benzaldehyde and malonic acid dihydrazyde in molar ratio 2:1 in methanol in the presence of perchloric acid, Cd(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O or Co(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O 5.5.11.11-tetraphenyl-5.6.11.12-tetrahydro-6.12-biiminodibenzo[b.f][1.5] diphosphonium diperchlorate (1) was obtained. We propose that malonic acid dihydrazide was subject of degradation to hydrazine under the experimental conditions, and that liberated hydrazine reacted with 2-(diphenylphosphino)benzaldehyde. In order to confirm the assumption reaction of 2-(diphenylphosphino)benzaldehyde and hydrazine sulfate in methanol at pH 1.5-2 in the presence of perchloric acid as catalyst was performed and 1 was obtained. 1 was characterized by IR and NMR spectroscopy and MS spectrometry. The probable reaction mechanism for this condensation involved aldehyde and hydrazine, which in situ form hydrazone, followed by addition of nucleophilic phosphorus to afford the final product. 1 possesses two positively charged nonmetal centers and structure similarly with dinuclear complexes of Cd(II), Co(III), Ni(II) and Zn(II) with  $N', N'^2$ -bis[(1E)-1-(2pyridyl)ethylidene]propanedihydrazide [1-4]. Such a compound is expected to show biological activity, because its positive charge would enable it to engage in electrostatic interactions with DNA. Additionally, absence of metal ions in the structure could lead to less pronounced toxicity. 1 showed a strong toxicity against brine shrimp with LC50 52.7 µM.

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P.S.E.2.

#### IN VITRO ANTITUMORAL ACTIVITY OF PLATINUM(IV) COMPLEX WITH 0,0'-DIPROPYL-(S,S)-ETHYLENEDIAMINE-N,N'-DI-2-(4-METHYL)PENTANOATE LIGAND

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Many platinum complexes have been synthesized not only in order to investi-gate their chemistry but also to identify novel compounds with improved antitumoral properties in comparison to the drug cisplatin [1,2]. Platinum(IV) complexes have greater inertness than corresponding platinum(II) complexes, thus allowing the oral administration and reducing the toxicity associated with platinum-based chemotherapy.

Here, we describe the synthesis, characterization and *in vitro* antitumoral activity of novel platinum(IV) complex: tetrachloro(*O*, *O'*-dipropyl-(*S*, *S*)-ethylenediamine-*N*, *N'*-di-2-(4-methyl)-pentanoate)platinum(IV). The reported platinum complex was discussed on the bases of infrared, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. In addition, citotoxicity on human colorectal adenocarcinoma cell line SW480 using MTT colorimetric assay [3] was reported. The complex was found to exhibit higher antitumoral activity than cisplatin on SW480 cell line.

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P.S.E.3.

## THE SWELLING BEHAVIOR OF THE POLY(METHACRYLIC ACID) HYDROGELS MODIFIED WITH DIFFERENT TYPE OF PECTIN

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The hydrogels based on crosslinked poly(methacrylic acid) and different type of pectin, were synthesized via free radical polymerization in aqueous media. The influence of the type and concentration of pectin on the equilibrium swelling degree was investigated. The initial formulation consists of methacrylic acid as monomer, potassium persulfate as initiator, 2-diethylamino ethanol as activator, N,N'-methylenebisacrylamide as crosslinker and pectin as linear polymer. Two series of pectin modified poly(methacrylic acid) hydrogels were synthesized. In the first series, hydrogels with different concentration of low amidated pectin (0-20 mol % respective to methacrylic acid) were prepared keeping constant concentration of monomer, crosslinker initiator and activator. In the second series low amidated pectin was substituted with high methyl-esterified pectin. The hydrogels were synthesized in closed vessels at 80 °C for 3 h, and were left to dry at ambient temperature, from which disks of diameter of 5 mm and thickness of 1.5 mm were taken, and used for swelling experiments at 25 °C. The results have shown that the amount of pectin added decreases the amount of absorbed water in the system, but that the decrease of water absorption is limited by the amount of pectin added, and variation of the type of pectin strongly influences the amount of swelling of hydrogels.

P.S.E.4.

#### NANOINDENTATION HARDNESS OF ENAMEL

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As the hardest and one of the most durable load-bearing tissues of the mammal bodies, enamel has attracted considerable interest from both material scientist and clinical practitioners due to its excellent mechanical properties. The nanoindentation was performed to observe the structure of enamel cross-sectioned to probing their mechanical properties. Orientation of enamel rods plays important role in mechanical behaviour of enamel. Their orientations were confirmed by AFM. The nanohardness and elastic modulus of the enamel from top to bottom region are significantly different. Both nanohardness and elastic modulus gradually decrease from enamel surface toward dentino-enamel junction. The results presented clarify the basic nanomechanical properties of human enamel and provide a useful reference for the future development of dental restorative materials.

P.S.E.5.

## PARAMAGNETIC NANOPARTICLES IN THE REGENERATION OF THE REDUCED ALVEOLAR BONE DENSITY

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One of the trends in the treatment of reduced bone density is in oral implantology through the use of new biomaterials with paramagnetic properties. In this in vivo study the effect of Ca / Co-HAp nanoparticles (calcium/cobalt-hydroxiapatite) in the regeneration of the reduced alveolar bone density in experimental animals was examined by analyzing both the biochemical and histochemical markers and through analysis of alveolar bone density. The research was carried out on female Westar rats, aged 6-8 weeks, whom have been implanted nanobiomaterial in reduced alveolar bone density. Good results in regeneration of reduced bone density were achieved in six weeks after implantation of the nanoparticles with paramagnetic properties. Biochemical markers of osteogenesis showed statistically significant rise. Histological analysis revealed high level reparatory skills of the biocomposite implanted in the bone defect, while x-ray analyses evidenced rise of bone density. Implantation of Ca/Co-Hap enables rapid new formation, thus becoming the material of choice for accelerated reduced bone density regeneration.

Keywords: biomaterials, nanoparticles Ca/Co-Hao, osteoporosis, alveolar bone, regeneration.

P.S.E.6.

## THE INFLUENCE OF INITIATOR TYPE ON THERMAL PROPERTIES OF SYNTHESISED POLY(L-LACTIDE)

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The growing pressure for resolving ecological problems makes bio-renewable and biodegradable materials, such as poly(lactide) very important. Over the past decade, the discovery of new polymerization routes which allow the economical production of poly(lactide) have resulted in an expanded use of this polymer for many applications (consumer goods, medical or pharmaceutical application). In this work different types of initiator were applied for polymerization of (3S)-cis-3,6-dimethyl-1,4-dioxane-2,5-dione (L-Lactide) to obtain poly(Llactide) (PLLA). For bulk polymerization performed in vacuum sealed vessel at 150 °C for 140 h the tin(II) 2-ethylhexanoate (Sn(Oct)<sub>2</sub>) was used as initiator. For solution polymerization the strong acid (trifluoromethanesulfonic acid) was used as initiator. In this procedure for very short period of time (less than 6 h) the obtained PLLA had narrow molecular weight distribution. Trifluoromethanesulfonic acid protonates monomeric lactide and propagation was preceded according to the activated monomer mechanism. The obtained polymers had a number-average molecular weights in the range from 50.000 to 218.000 (polydispersity index from 1 to 3, depending on the initiator types) according to gel permeation chromatography measurements. Thermal properties of synthesized polymers were investigated using differential scanning calorimetry and thermogravimetric analysis. The presence of -OH and -C(O)OSO<sub>2</sub>CF<sub>3</sub> endgroups in polymers obtained in the presence of trifluoromethanesulfonic acid allowed efficient end-to-end cyclization which results in higher thermal stability. It was estimated that degradation onset temperature of polymers with -C(O)OSO<sub>2</sub>CF<sub>3</sub> end-groups (synthesized with trifluoromethanesulfonic acid as initiator), was much higher than degradation temperature of linear poly(L-lactide) (synthesized in the presence of Sn(Oct)<sub>2</sub>).

P.S.E.7.

#### AGGREGATION OF FULLERENOL NANO PARTICLES IN CELL MEDIUM RPMI 1640 WITH FETAL BOVINE SERUM

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The aim of this research was to investigate aggregation of fullerenol C<sub>60</sub>(OH)<sub>24</sub> nano particles (FNP) of different concentrations in RPMI 1640 cell medium with fetal bovine serum (FCS) at 37°C after incubation period of 4h and 24h. Water-soluble polyhydroxylated derivates of fullerene - fullerenols ( $C_{60}(OH)x$ : x=12–26) showed various biological functions. Fullerenol C<sub>60</sub>(OH)<sub>20</sub> expresses immunomodulatory activity on immune cells, such as T-cells and macrophages-both in vivo and in vitro, as well as improves the immune response and so helps scavenging and killing tumor cells. FNP is a mitochondrial protective antioxidant with direct radical scavenging activity and indirect antioxidant inducing activity. Atomic Force Microscopy (AFM) studies compared characteristics of FNP in: water solution, RPMI 1640 + 17% FCS, RPMI 1640 + FCS 24%, after incubation of 4h and 24h at 37°C. AFM analysis of water solution of FNP, performed on highly orientated pyrolytic graphite (HOPG), resulted in homogenous distribution of particles with diameter of 80-90 nm. DLS measurements of the distribution number of FNP, confirmed the dominant presence of particles with diameter of 90 nm, and a small percentage of particles sizing between 20-30 nm. After 24h at 37°C FNP in RPMI 1640 + FCS25%, particles of about 180 nm in diameter were formed, which consisted of two particles of 90 nm and a particle of 44 nm. Similar results were obtained by AFM analysis of FNP in RPMI +17% FCS after 4h and 24h. The results obtained by DLS measurements of FNP in RPMI +25% FCS indicated that dimensions of nano particles were 185, 93 and 40 nm. Incubation of FNP in presence of RPMI 1640 with FCS at 37°C for 24h significantly changed characteristics and distribution of nano particles. FNP with FCS proteins formed a homogeneous particle system (FNP particles + protein) of about 180 nm. The studies of aggregation of FNP in cell medium are expected to be helpful for better understanding the complex biological mechanisms of FNP activities at the cellular level.

P.S.E.8.

#### BIOLOGICAL ACTIVITIES AND PHYTOCHEMICAL SCREENING OF THE PLANT KITAIBELIA VITIFOLIA

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The objective of this study was to evaluate the potential use of essential oil of K. vitifolia in the pharmaceutical and food industries. Antimicrobial and antioxidant activities of essential oil of K. vitifolia isolated by hydrodistillation using Clevenger-type apparatus were assessed. GC/FID and GC/MS analyses were used to determine the following major components of K. vitifolia essential oil: sclareoloxide (cis A/B) 17.9 %, sclaral 10.9 %, labda-7,13,14-triene 10.6 % and sclareol 9.5 %. The antimicrobial activity of the essential oil was evaluated against the bacterial strains: Staphylococcus aureus ATCC 25923, Klebsiella pneumoniae ATCC 13883, Escherichia coli ATCC 25922, Proteus vulgaris ATCC 13315, Proteus mirabilis ATCC 14153, Bacillus subtilis ATCC 6633; and fungal strains: Candida albicans ATCC 10231 and Aspergillus niger ATCC 16404. Antimicrobial activity was tested using broth dilution procedure for determination of minimum inhibitory concentration (MIC). The essential oil of K. vitifolia showed a strong antimicrobial activity. Antioxidant activity was determined by 2, 2-dephenyl-1picrylhydrazyl (DPPH) free radical scavenging assay. The results on antioxidant activity were compared with control antioxidants, ascorbic acid and BHT. The IC<sub>50</sub> values determined for each measurement were 7.81, 5.99, 12.77 µg/ml for essential oil, ascorbic acid and BHT, respectively, for DPPH free radical scavenging.

Keywords: Kitaibelia vitifolia, essential oil, antimicrobial and antioxidant activities.

P.S.E.9.

## BIODEGRADABLE CITRIC-ACID BASED POLYESTER ELASTOMERS FOR TISSUE ENGINEERING APPLICATIONS

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The synthesis and fabrication of polyester elastomers using non-toxic and biocompatible reactants is a topical research area in tissue engineering applications. In such applications, a primary role of the material is to interface with the biological system to treat or replace any organ or functional tissue of the body. The most important feature of such synthetic biomaterials is their controllable structural integrity that strongly influences interfacial behaviour in biological environment. In order to investigate the interfacial phenomena of synthetic polyester elastomers, we have successfully developed a simple synthesis of such unique elastomer by carrying out catalyst-free polyesterification of multifunctional non-toxic monomers: 1,8octanediol (OD), citric acid (CA) and sebacic acid (SA). The chemical, physical, structural and surface chemical properties of the resulting co-polyester polyoctanediol citrate/sebacate [p(OCS)] have been investigated. We demonstrate that the chemical structure, morphology, physical integrity and surface chemistry of the synthesized co-polyester can be controlled by simply varying the initial acid concentration (CA/SA) in reaction mixture. This research provides useful approach for tailoring fundamental properties of the biocompatible elastomers that have significant potential for tissue engineering applications. The investigation results of in vitro biological response of human-derived osteoblast-like cells (MG63) to p(OCS) elastomers will also be presented.

P.S.E.10.

# HYDROTHERMAL SYNTHESIS OF ZnO NANOSTRUCTURES WITH DIFFERENT MORPHOLOGIES AND THEIR ANTIMICROBIAL ACTIVITY AGAINST Escherihia coli AND Staphylococus aureus BACTERIAL CULTURES

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Considering that many very important properties that determine the use of material for a range of purposes depend on size and morphology of the particles of which the material is made up of exceptional importance is the synthesis of particles of controlled morphology and dimensions. Nanoparticle metal oxides represent a new class of important materials that are increasingly being developed for use in research and health-related applications. Zinc oxide is currently being investigated as an antimicrobial agent in both microscale and nanoscale formulations. Results have indicated that ZnO nanoparticles show antibacterial activity apparently greater than for microparticles. In this study, we generally attempt to examine influence of size and particularly shape of ZnO nanoparticles synthesized through a controlled hydrothermal method, on the antibacterial activity toward *Escherihia coli* (Gram-negative bacteria) and *Staphylococcus aureus* (Gram-positive bacteria).

Characterization of the prepared ZnO nanopowders was performed using experimental technique such as XRD analysis, FE SEM, HR TEM, UV VIS and Malvern's Master Sizer instrument for particle size distribution. The antibacterial properties of synthesized ZnO nanostructures were done using a colony count method.

Apart from different forms of prepared ZnO nanoparticles, antimicrobial tests showed impressive antibacterial properties, above 99% microbial cells reduction, toward gram positive bacteria *S. Aureus* and gram negative bacteria *E. Colli*.

#### P.S.E.11.

#### CHITOSAN-POLYETHYLENE OXIDE FILMS FOR CONTROLLED DRUG RELEASE

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This report presents the fabrication of polymer films based on chitosan and polyethylene oxide (PEO) and the ability of films to tune drug release. Film thickness varied between 353 and 409 µm depending on the PEO content. Crystallinity of the polymer mostly depent of the increase of PEO as shown by DSC, XRD and optical microscopy Water contact angle decreased from pure chitosan to 50/50 wt% chitosan/PEO and then increased with increasing the PEO content, which is attributed to the formation of partially ordered crystalline structure. The addition of PEO induced the increase of swelling degree, which is in agreement with results of water contact angle measurements. Release rate of paracetamol drug decreased with the addition of PEO due to increased crystallinity and coherent structure of the film. A faster release of paracetamol from the pure chitosan film was observed due to the presence of meso-and macropores in examined films after swelling.

P.S.E.12.

## THE FABRICATION OF ELECTROSPUN CHITOSAN NANOFIBER'S MAT WITH EMBEDDED SINGLE- AND MULTI-WALLED CARBON NANOTUBES

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Oxidized single and multiwalled carbon nanotubes were embedded in chitosan-polyethylene oxide matrix with the addition of sodium cholate as a surfactant. The mat of composite nanofibers was fabricated by electrospinning process. The nanofiber morphology, thermal stability and composition were examined by HRTEM, TGA and DSC. The optimal composition of chitosan and PEO as well as the addition of biocompatible surfactant sodium cholate yielded biocompatible nanofibers with uniform diameter by decreasing the solution viscosity. Incorporation of carbon nanotubes increased the functionality potential and mechanical properties of electrospun fibers' web with faster electron transfer kinetics thus enabling its implementation in biological areas and in photovoltaic applications.

P.S.E.13.

## MONOMER ELUTION FROM EXSPERIMENTAL COMPOSITES WITH HYDROXYAPATITE FILLERS

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Resin based composite materials (RBCs) generally consist of resin matrix, inorganic fillers and a silane coupling agent. Monomer conversion to polymer in RBCs is incomplete. Unreacted monomers are trapped in the polymer matrix and may elute from RBCs. Elution of monomers from RBCs may adversely affect the biocompatibility and mechanical properties of these materials. Studies on the biocompatibility of monomers showed allergenic, cytotoxic, genotoxic and estrogenic effects of these substances. The aim of this study was to determine elution of monomers TEGDMA and BisGMA from experimental composites with hydroxyapatite (HAP) fillers. Four experimental composite materials were investigated. Groups 1-3 contained 80:20 wt% fillers to resin ratio and this ratio was 75:25 wt% in group 4. Group 1 had only conventional mixed oxide fillers with no HAP. In group 2, 10% and in groups 3 and 4, 20% of conventional filler were replaced with HAP particles. One commercial microhybrid composite was used as control. Five samples of each material were prepared in standardized Teflon molds. Eluted monomers were quantified using high performance liquid chromatography (HPLC) after storage in 75% ethanol/water solution for 7 days. Material composition significantly affected the amount of eluted monomers. Experimental composite material with 10% HAP showed lower elution of monomers than the commercial material.

#### THIRTEENTH ANNUAL CONFERENCE YUCOMAT 2011

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P.S.E.14.

#### STRESS-STRAIN RELATIONS BETWEEN POLYMER GEL MICROENVIRNMENT AND GOWING CELL CLUSTERS

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Rheological properties of complex systems, in particular encapsulated living cell systems in polymer matrix require special approaches to basic constitutive relations. Moreover, mechanical quantities such as stress and strain in tissue can modulate its growth, what is of high importance for biomaterial application and medical engineering in general. A number of authors considered growth and remodeling of bone and cartilage under different rheological conditions. But for such dynamical systems as cell clusters encapsulated inside soft polymer gels is difficult to apply formal methods from mechanics that require reference state for stress measurements.

In this contribution is considered the concept of virial stress application to complex rheological systems described. The stress includes two parts. The first depends on mass and velocity of particles, reflecting an assertion that grow of cluster causes mechanical stress to be applied on polymer surface external to particle system. The second part depends on interaction forces and cell dynamics e.g. cell positions, providing continuum interactions between particles making the cluster. Statistical mechanical methods will be applied to average contributions of individual cells

#### P.S.E.15.

#### CHARACTERIZATION OF FULLERENES THIN FILM ON GLASSES AND CONTACT LANCES BY UV/VIS /IR AND OPTO-MAGNETIC SPECTROSCOPY

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UV/VIS investigation of glasses and contact lances is part of standard procedure. Reason for to do it is to protect eyes from UV and characterized material from transparence. However, we extend this research to IR domain because quality of glasses and contact lances depend not only from UV protection and its transparence but from complementarities and compatibility of eyes vision with optical device.

We characterized basic material of glasses and contact lances by UV/VIS/IR and OMS. Than we doped both basic materials with fullerenes, and using same procedure characterized them. Also, comparative investigation by OMS was done. Results are presented and discussed.

P.S.E.16.

## AFM/MFM INVESTIGATION OF FULLERENES THIN FILM ON GLASSES AND FULLERENE DOPED CONTACT LANCES

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Optical signal is very important for both human vision (nerve pathways from the eyes to the brain) and deeper brain areas concerned with neurotransmiters, neurohormones, emotions, etc. In current ophthalmology research only integral electromagnetic signal is considered. However, experimental results strongly indicate that electrical and magnetic signals are different when eyes are close and open. This indicates that type of material of glasses and contact lances from electrical and magnetic properties is important.

In this work we have carried out the research of fullerenes nano films on glass and contact lenses doped fullerenes ( $C_{60}$  molecule) and fullerene added forms  $C_{60}$  (OH)  $_{24}$  by AFM (Atomic Force Microscopy) and MFM (Magnetic force Microscopy). We present difference on nanoscale between basic material of contact lances and doped ones. Also, we compared current MFM results of nano films with previous our research based on remnant magnetization. It has been shown that glasses based on nano films change human EEG signals. Current research is in progres.

P.S.E.17.

## pH SENSITIVE COPPER/POLY(2-HYDROXYETHYL ACRYLATE/ITACONIC ACID) HYBRID HYDROGELS

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The novel copper/poly(2-hydroxyethyl acrylate/itaconic acid) (Cu/P(HEA/IA)) hybrid hydrogels were successfully prepared by free radical crosslinking copolymerization of 2-hydroxyethyl acrylate (HEA) and itaconic acid (IA), with the subsequent embedding of Cu(II)-ions by swelling the hydrogels in the copper salt solution. Itaconic acid, diacid derived from natural sources, was used as a component which improves biomedical performances of a polymeric biomaterial. Copper ions are also of biomedical importance due to their angiogenic and wound healing properties. Therefore, hydrogels containing IA and copper ions behave as multifunctional biomaterials.

Structure and morphology of the samples were characterized by Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). FTIR measurements confirmed the presence of copper ions in the hydrogel network. Morphology examination showed a heterogeneous distribution of copper ions in the Cu/P(HEA/IA) hybrid hydrogels.

Swelling studies were performed in a wide range of physiologically important pH and temperature values in order to mimic living tissue conditions. The results showed pH sensitive behavior of Cu/P(HEA/IA) hybrid hydrogels with a maximum swelling at pH 6.0. Embedding of Cu(II)-ions had no significant influence on pH behavior of P(HEA/IA) hydrogels, but temperature sensitiveness disappeared. Swelling kinetic parameters indicated a Fickian fluid transport. The obtained results confirmed that such a new type of Cu-ion loaded hybrid hydrogels may be considered as good candidates for biomaterials in biomedical/therapeutic applications.

P.S.E.18.

## THE EFFECT OF REACTION CONDITIONS ON BASIC STRUCTURAL PARAMETERS AND ELECTRICAL CONDUCTIVITY OF POLY(ACRYLIC ACID)-GELATIN COMPOSITE HYDROGELS

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This paper reports on the influence of reaction conditions on the basic structural parameters and electrical conductivity of poly(acrylic acid)-gelatin (AA-G) composite hydrogels. The composite hydrogels were synthesized via free-radical polymerization and crosslinking in an aqueous solution. An 2,2'-azobis-[2-(2-imidazolin-2-yl)propane] dihydrochloride (VA-044) was used an initiator and N,N'-methylene bisacrylamide (MBA) as a crosslinker. The main goal was to find corelationship between the reaction conditions (crosslinker concentration ( $C_{MBA}$ ) and degree of neutralization of acrylic acid ( $ND_{AA}$ )), basic structural parameters and electric conductivity of the synthesized hydrogels.

The basic structural parameters (average molar mass between the network crosslinks ( $M_c$ ), crosslinking density ( $\rho_c$ ), and distance between macromolecular chains ( $\xi$ )) were calculated by Flory and Rehner equation. The obtained results showed that the reaction conditions significantly influence the structural properties of hydrogles. The increase of  $C_{MBA}$  leads to the decrease of the  $SD_{eq}$ ,  $M_c$  and  $\xi$ , while the  $\rho_c$  increases. On the other hand, equilibrium swelling degree ( $SD_{eq}$ ),  $M_c$  and  $\xi$  increase with increasing  $ND_{AA}$ , while the  $\rho_c$  decreases. It was found that electrical conductivity of the samples decrease with decreasing crosslinker concentration and degree of neutralization of acrylic acid.

P.S.E.19.

## ELECTRODE-SKIN INTERFACE MODIFICATION: HYDRATION AND IONIC STRENGTH EFFECT

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Different biomedical surface electrodes are placed on the skin in order to distribute or collect electrical or chemical stimulus and consequently induce or detect relevant biomedical event. The intimate contact between electrode and outer skin layer often called electrode-skin interface is considered to be a principal barrier for stimulus delivery and detection. Skin in general behaves as a responding membrane and it is known that minor change in skin environment can lead to change in its barrier properties. Well established criteria that determine desirable properties of transcutaneous electrodes are well defined impedance, homogenous current distribution, flexibility that allows electrode to adopt given body curvature and maintain good contact, facile application and removal and absence of skin irritation. In this study, we have investigated the effect of change in electrode-skin interface hydration and electrolyte ionic strength on its electrical barrier properties. Impedance spectroscopy measurements were performed on pig skin in vitro. The skin samples investigated were exposed to a hydrophilic polymer (polyethylene oxide) and salt (NaCl) solutions and were compared with skin samples in physiological conditions. Bacterial cellulose was used as a model system with less complex structural and chemical composition than skin. Our experimental findings indicate preferred pathways for electrical current crossing the electrode-skin interface and provide insight into the related method to establish better control over interface barrier properties.

P.S.E.20.

## INFLUENCE OF PRODUCTION TECHNIQUES ON ELECTROCHEMICAL PROPERTIES OF THE Mg-3Al-1Zn ALLOY IN BODY-FLUID SOLUTION

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The electrochemical characteristics of a biodegradable magnesium alloy in simulated bodyfluid (Hank's solution) were investigated. The experiments were done on magnesium alloy containing the aluminium and zinc as main alloying elements after two various production techniques – die casting and extrusion. The differences in microstructures were evaluated by light microscopy. Extruded microstructure is finer (with average grain size of ~17  $\mu m$ ) in comparison with coarse grained microstructure of as cast alloy (~200  $\mu m$ ). The electrochemical impedance spectroscopy method in combination with exposure (immersion) tests was used for determination of the electrochemical characteristics. The electrochemical characteristics were determined after various times (5 min., 1, 2, 4, 8, 16, 24, 48, 96, 168, 336 and 504 hours) and the Nyquist plots as results of electrochemical impedance spectroscopy were analysed using two various types of equivalent circuits. The results of electrochemical tests were supplemented by light microscopy of attacked surfaces. The measured results show that the finer microstructure of the alloys leads to the more uniform corrosion process in physiological solution.

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P.S.E.21.

## THE ROLE OF PERIFERAL BLOOD CELLS IN THE INDUCTION OF ECTOPIC OSTEOGENESIS

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The bone marrow is a rich source of cells for assisted bone reparation. It contains adherent stromal stem cells (CFU-f) that can differentiate into various connective tissues including bone, cartilage, fat and fibrous tissue. Also, there is more data about the existence of nonadherent cells in the peripheral blood that have characteristics of stem and/or osteoprogenitor cells. Since the procedure of blood taking is easy, safe and can be repeated many times on the same patient, it is possible to use these cells in bone regeneration.

The aim of our research was to examine whether and to what extent cells of whole blood in combination with the bone mineral matrix has an impact on the induction of ectopic osteogenesis.

The study was conducted on syngene BALB/c mice, male, 10-12 weeks old. Implants were obtained by mixing the bone mineral matrix with whole blood, and bone mineral matrix with physiological solution. Subcutaneus interscapular implantation was performed and the animals were sacrificed after 1, 2 and 4 weeks after implantation. Hematoxylin-eosin and Masson's trichrome stainings were used for histological evaluation.

Both types of implants showed chemotaxis effect to different connective tissue cells and osteoclasts but they didn't show significant osteoinduction. The bone mineral matrix showed a better stimulatory effect on these processes compared to combination of mineral matrix and whole blood cells.

These results suggest that bone mineral matrix alone has better osteoinductive potential than whole blood in combination with bone mineral matrix.

Keywords: bone mineral matrix, blood cells, ectopic osteogenesis.

P.S.E.22.

#### SOLID STATE PROPERTIES AND ANTICANCER EFFECTS OF ARSENIC SULPHIDE NANOSUSPENSIONS

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In this study, arsenic sulphide  $As_4S_4$  nanoparticles have been prepared, by nanomilling, in the presence of sodium dodecylsulphate, which acts as a surfactant. For nanomilling, the laboratory Perl Mill PML2 (Bühler) has been used. Solid state properties of the nanoparticles were characterized by surface area, particle size distribution and  $\xi$ -potential measurements. Changes in specific surface areas of the particles, in the 0.2-34.2 m²/g range, nanosized monomodal distributions, in the 40-387 nm range and  $\xi$ -potential values in the -52 to -38 mV range, characterise the surface and morphological properties of arsenic sulphide nanoparticles. Dissolution experiments in simulated gastric fluid (HCl + NaCl + pepsin) show a possibility for the application of the realgar nanoparticles as an oral dose in future arsenic drug cancer treatment.

P.S.E.23.

## SYNTHESIS OF CORE-SHELL PARTICLES WITH BOTH FERITE AND SILICA SHELL AS SUPPORTS FOR ENZYME IMMOBILIZATION

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Monodispersed and spherical silica core particles synthesized by hydrolysis and condensation of tetraethilortosilicate and having average size of ~0.5  $\mu$ m were used as templates for formation of ferrite and silica nanoshells. In the first step, ferrite shell was formed around silica core by attractive electrostatic assembling of ferrite nanoparticles. In the second step, silica nanoparticles were synthesized by acidic neutralization of highly basic sodium silicate solution and than precipitated on previously functionalized silica core/ferrite shell particles. Synthesized bilayered core-shell particles are superparamagnetic due to existance of Fe<sub>3</sub>O<sub>4</sub> nanoshell with average shell thickness of ~50 nm. However, average pore size and total pore volume of ferite shell are small which make them unsuitable for enzyme immobilization but good for magnetic separation of core-shell particles from reaction medium. On the other side, mesoporous silica shell which exists on the surface of ferrite shell has large pore volume and pore size which allow enzyme immobilization inside mesoporous shell.

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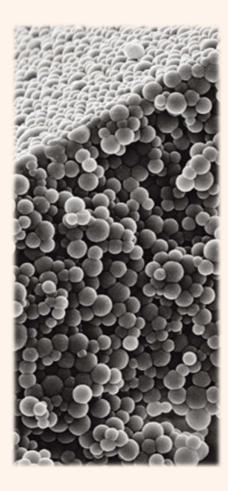
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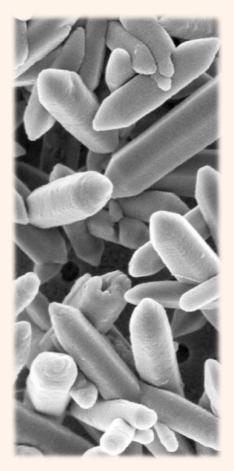
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