

TWELFTH ANNUAL CONFERENCE

YUCOMAT 2010

Hotel "Plaža", Herceg Novi, Montenegro, September 6–10, 2010
<http://www.mrs-serbia.org.rs>



Programme and The Book of Abstracts

Organised by:

Materials Research Society of Serbia
and

**Institute of Technical Sciences of the
Serbian Academy of Sciences and Arts, Belgrade**

under the auspices of

Federation of European Materials Societies (FEMS)

and

Materials Research Society (MRS)

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Title: THE TWELFTH ANNUAL CONFERENCE
“YUCOMAT 2010”
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WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA

Dear Friends and Colleagues, Welcome to YUCOMAT 2010 Conference and the fabulous town of Herceg-Novi!



This year we are celebrating 15 years from the first YUCOMAT Conference, which was held in this very venue in 1995. The Conference initiated the formation of the Yugoslav Materials Research Society, which was a decade or so later renamed to Materials Research Society of Serbia. During the last 15 years, the quality of the Conference, the number and the diversity of the exciting plenary lecturers coming from a variety of scientific centres from all over the globe has steadily grown. As can be expected, the 2010 Conference has some new records to set.

Those exist in terms of the so far unprecedented 4 plenary sessions, 25 invited lectures which will be held by some of the world-renowned experts in their fields, 5 symposia with 5 oral and 3 poster sessions, and 259 presentations overall. The participants of this year's Conference come from 36 countries of the world. We all know how small our MRS is compared to other similar societies of the world and how great of an achievement this could be taken as. This sheds new light on the slogan given for a few past YUCOMAT conferences: “Small is beautiful”.

This year's participants will have a chance to attend presentations on some of the most exciting topics of Materials Science that currently stand on the frontier of the field. Nanostructured materials and thin films, biomaterials for a variety of applications, functional bio-nano-interfaces, structural simulation and modelling, cutting-edge methods for probing materials structure, morphology and various mechanical and spectroscopic properties at the atomic scales, advanced materials applicable in high-tech devices and a plethora of new synthesis methods that offer sophisticated control over materials' properties on various scales are some of the topics that will be discussed during the Conference. Apart from a plenty of interesting lectures, the participants will have a chance to lighten up and communicate in friendly and relaxed settings. As every time before, we have made sure to provide you with a lot of such opportunities. The traditional Photo Session and the Welcome Cocktail on Monday, the Poster Sessions on Tuesday, Wednesday and Thursday evenings, a trip to Dubrovnik on Wednesday afternoon, a boat trip around the Bay on Thursday afternoon, and numerous coffee breaks will present some of these informal occasions for socializing and networking.

To maintain the tradition of scientific excellence in the field, we are giving awards to some of the most prospective young researchers for their achievements. Hence, awards for the best doctoral and master theses defended between the two Conferences will be given as well as those for the best oral and poster presentations.

Our Presidency and the Organizing Committee, with the help from the International Advisory Board and Aleksandra Stojičić, the Conference Secretary, worked hard to put this meeting together. I would like to particularly thank our Vice-Presidents, Drs. Velimir Radmilović, Dejan Raković and Slobodan Milonjić, for their invaluable suggestions and an enthusiastic support, especially in promoting the MRS-Serbia and attracting scientists of an impressive background as plenary speakers.

On behalf of the MRS-Serbia officers, I wish this to be yet another splendid YUCOMAT conference filled with many refreshing and memorable moments.

Dragan Uskoković

MRS-Serbia

President: Dragan Uskoković

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

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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).

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Programme

**TWELFTH ANNUAL CONFERENCE
"YUCOMAT 2010"
Herceg Novi, September 6-10, 2010**

CONFERENCE PROGRAMME

- SYMPOSIUM A** Advanced Methods in Synthesis and Processing of Materials
SYMPOSIUM B Advanced Materials for High-Technology Application
SYMPOSIUM C Nanostructured Materials
SYMPOSIUM D Composites
SYMPOSIUM E Biomaterials

GENERAL INFORMATION

DATE AND VENUE: The conference will be held on September 6-10, 2010, at the Plaža Hotel, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 6, at 09.00 and end on Friday, September 10th, 2010 at 12.00.

REGISTRATION: Registration, registration fee payment, conference materials distribution, etc. will take place at the conference desk (Conference Secretariat) open on Sunday, September 5, Monday, September 6, and Tuesday, September 7, 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.

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 only, 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 Business Club (next to the National Restaurant, looking at the beach) which is open Tuesday to Thursday 18.00-22.00.

PUBLICATION OF PAPERS: Abstracts will be included in a book of abstracts and distributed to each participant at registration. Only the papers presented at the Conference will be peer reviewed and, if positive, selected papers will be published in the International Journal of Modern Physics B (by World Scientific, IF 0.408, <http://ejournals.wspc.com.sg/ijmpb/mkt/guidelines.shtml>), on SCI list. Manuscripts prepared according to the guidelines for this journal, which are of good quality, comprehensible English language and with more than 50% references from the last 5 years, will have advantage. Detailed instructions for preparation of manuscripts are available on the website given above.

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.

GENERAL CONFERENCE PROGRAMME

Sunday, September 5, 2010

08⁰⁰-19⁰⁰ **Registration**

Monday, September 6, 2010

08⁰⁰-09⁰⁰ **Registration**
09⁰⁰ **OPENING CEREMONY**
- Introduction and Welcome

10⁰⁰-13⁰⁰ **First Plenary Session**
13³⁰ **Photo Session**
15⁰⁰-19¹⁵ **Symposium A, Conference Hall**
15⁰⁰-19⁰⁰ **Symposium B, Press Hall**
19³⁰-21⁰⁰ **Cocktail Party**

Tuesday, September 7, 2010

09⁰⁰-13³⁰ **Second Plenary Session**
15⁰⁰-19⁰⁰ **Symposium C, Conference Hall**
15⁰⁰-19⁰⁰ **Symposium D, Press Hall**
20³⁰-22⁰⁰ **Poster Session I (Symposium A)**

Wednesday, September 8, 2010

09⁰⁰-13⁰⁰ **Third Plenary Session**
14⁰⁰-19⁰⁰ **Excursion to Dubrovnik, Croatia**
20³⁰-22⁰⁰ **Poster Session II (Symposium B)**

Thursday, September 9, 2010

09⁰⁰-12³⁰ **Fourth Plenary Session**
14⁰⁰-19⁰⁰ **Boat-trip around Boka Kotorska Bay**
20³⁰-22⁰⁰ **Poster Session III (Symposiums C, D and E)**

Friday, September 10, 2010

09⁰⁰-11³⁰ **Symposium E**
11³⁰-12⁰⁰ **Awards and Closing of the Conference**

SYMPOSIUM A: Advanced Methods in Synthesis
and Processing of Materials
SYMPOSIUM B: Advanced Materials for High-
Technology Application
SYMPOSIUM C: Nanostructured Materials
SYMPOSIUM D: Composites
SYMPOSIUM E: Biomaterials

FIRST PLENARY SESSION

Monday, September 6, 2010

Session I: 10⁰⁰-13⁰⁰

Chairpersons: R. Siegel, V. Radmilović and R. Sinclair

Conference Hall

10⁰⁰-10³⁰ **A LOOK AT NANOTECHNOLOGY: PAST, PRESENT, FUTURE**
R.W. Siegel
*Materials Science and Engineering Department, Rensselaer Nanotechnology Center,
Rensselaer Polytechnic Institute, Troy, New York, USA*

10³⁰-11⁰⁰ **THE IMPACT OF TRIPLE LINES ON MATERIALS SCIENCE AND
ENGINEERING**
A.H. King
The Ames Laboratory, Ames, IA, USA

11⁰⁰-11³⁰ **BIO-INSPIRED STRUCTURAL MATERIALS**
R.O. Ritchie
*Department of Materials Science & Engineering, University of California Berkeley,
and Materials Sciences Division, Lawrence Berkeley National Laboratory, CA, USA*

Break: 11³⁰-12⁰⁰

12⁰⁰-12³⁰ **RECENT ELECTRON MICROSCOPE STUDIES OF GOLD-BASED
NANOPARTICLES FOR MEDICAL APPLICATIONS**
R. Sinclair, P. Kempen, A.L. Koh
*Department of Materials Science and Engineering and Stanford,
Nanocharacterization Laboratory, Stanford University, Stanford, CA, USA*

12³⁰-13⁰⁰ **CONVERGING THEORY AND EXPERIMENT: NUCLEATION OF L₁₂
COMPLEX NANOSTRUCTURES**
V. Radmilović
*Lawrence Berkeley National Laboratory, University of California, Berkeley, CA,
USA*

Break: 13⁰⁰-15⁰⁰

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

Monday, September 6, 2010

Session I: 15⁰⁰-19¹⁵

Chairmen: J. Kusinski and T. Shakhshneider

Conference Hall

- 15⁰⁰-15¹⁵ **INFLUENCE OF IRRADIATION DEFECTS ON THE STRENGTH OF
COPPER AT A NANOMETER SCALE**
D. Kiener^{1,2}, P. Hosemann^{3,4}, A.M. Minor^{2,4}
*¹Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben,
Austria, ²National Center for Electron Microscopy, Lawrence Berkeley National
Laboratory, CA, USA, ³Materials Science & Technology, Los Alamos National
Laboratory, Los Alamos, NM, USA, ⁴University of California, Berkeley, CA, USA*
- 15¹⁵-15³⁰ **STRUCTURE PREDICTION FOR PbS AND ZnO AT DIFFERENT
PRESSURES AND VISUALIZATION OF THE ENERGY LANDSCAPES**
D. Zagorac, J.C. Schön, K. Doll, M. Jansen
Max Planck Institute for Solid State Research, Stuttgart, Germany
- 15³⁰-15⁴⁵ **HIGH-TEMPERATURE OPTICAL IN-SITU STUDIES OF REDOX
PROCESSES IN COMPLEX OXIDES**
J. Shi, S. Duglocz, K.-D. Becker
*Institute of Physical Chemistry, Technische Universität Braunschweig,
Braunschweig, Germany*
- 15⁴⁵-16⁰⁰ **MECHANOCHEMICAL PREPARATION OF ORGANIC-INORGANIC
HYBRID MATERIALS OF DRUGS WITH INORGANIC OXIDES**
T.P. Shakhshneider^{1,2}, S.A. Myz^{1,2}, M.A Dyakonova², V.V. Boldyrev^{1,2}, E.V.
Boldyreva^{1,2}, R. Kumar³
*¹Institute of Solid State Chemistry and Mechanochemistry, SB RAS, Novosibirsk,
Russia, ²Research and Education Centre "Molecular Design and Ecologically Safe
Technologies" at the Novosibirsk State University, Novosibirsk, Russia, ³National
Metallurgical Laboratory, Jamshedpur, India*

16⁰⁰-16¹⁵ **REGULARITIES OF FORMATION, STRUCTURE AND CHEMICAL PROPERTIES OF NANOSIZED MoO₃ AND Me/MoO₃ (Me=Al, Mg, Si) NANOCOMPOSITES, PREPARED BY MECHANOCHEMICAL METHOD**
A.N. Streletskii¹, I.V. Kolbanev¹, A.Ju. Dolgoborodov¹, V.V. Artemov², A.V. Leonov³, A.B. Borunova¹
¹*N.N.Semenov Institute of Chemical Physics RAS, Moscow, Russia*, ²*A.V.Shubnikov Institute of Crystallography RAS, Moscow, Russia*, ³*Moscow State University, Chemical Department, Leninskie gory, Moscow, Russia*

16¹⁵-16³⁰ **BULK AMORPHOUS CU- AND NI- BASED ALLOYS PROCESSED BY MECHANICAL ALLOYING AND POWDER COMPACTION**
D. Oleszak, T. Kulik
Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland

16³⁰-16⁴⁵ **SYNTHESIS AND CHARACTERIZATION OF NiMn_xFe_{2-x}O₄ FERRITES**
S.M. Busurin, M.L. Busurina
Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow region, Russia

16⁴⁵-17⁰⁰ **SINTERING OF DEFECT-FREE BTS2.5/BTS5/BTS7/BTS10 FUNCTIONALLY GRADED MATERIALS**
S. Marković¹, S.D. Škapin², D. Suvorov², D. Uskoković¹
¹*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia*, ²*Jožef Stefan Institute, Ljubljana, Slovenia*

Break: 17⁰⁰-17³⁰

17³⁰-17⁴⁵ **MICROWAVE ASSISTED SOLVENT FREE REACTIONS OF SOME INTERCALATIVE COMPOUNDS AND PHTHALOCYANINE DERIVATIVES**
A.N. Mikheev
Nikolayev Institute of Inorganic Chemistry SB RAS, Novosibirsk; Research and Educational Centre, Research and Educational Complex, Novosibirsk State University, Russia

- 17⁴⁵-18⁰⁰ **PREPARATION OF LiFePO₄/C COMPOSITES BY CO-PRECIPIATION IN THE PRESENCE OF STEARIC ACID**
D. Jugović¹, M. Jović¹, M. Mitrić², N. Cvjetičanin³, D. Uskoković¹
¹*Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia,* ²*Vinča Institute of Nuclear Sciences, Belgrade, Serbia,* ³*Faculty of Physical Chemistry, University of Belgrade, Serbia*
- 18⁰⁰-18¹⁵ **PREPARATION AND SURFACE PROPERTIES OF CeO₂-Nb₂O₅ MIXED-OXIDE CATALYSTS**
D. Stošić¹, V. Rakić², S. Bennici¹, A. Auroux¹
¹*IRCELYON, UMR5256 CNRS- Université Lyon1, Villeurbanne, France,* ²*Faculty of Agriculture, Department of Chemistry, University of Belgrade, Zemun, Serbia*
- 18¹⁵-18³⁰ **PHOTOCATALYTIC ACTIVITY OF PHOSPHATED TiO₂ NANOPOWDERS**
V. Žunič, S.D. Škapin, M. Maček-Kržmanc, D. Suvorov
Jožef Stefan Institute, Advanced Materials Department, Ljubljana, Slovenia
- 18³⁰-18⁴⁵ **HIGH VELOCITY SUSPENSION FLAME SPRAYING (HVSFS); PROCESS DEVELOPMENT AND INDUSTRIAL APPLICATIONS**
A. Killinger, R. Gadow
Institute for Manufacturing Technologies of Ceramic Components and Composites (IMTCCC), University of Stuttgart, Stuttgart, Germany
- 18⁴⁵-19⁰⁰ **SUPERELASTIC BEHAVIOUR OF LASER WELDED JOINTS IN NiTi**
L. Alberty Vieira¹, F.M. Braz Fernandes², R.M. Miranda¹
¹*UNIDEMI, Departamento de Engenharia Mecânica e Industrial, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal,* ²*CENIMAT/13N, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal*
- 19⁰⁰-19¹⁵ **La_{1-x}Ca_xFeO₃ HOMOGENEOUS AND MICROHETEROGENEOUS PEROVSKITE-LIKE OXIDES: SYNTHESIS, MICROSTRUCTURE, STABILITY AND CATALYTIC ACTIVITY**
L.A. Isupova
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

Monday, September 6, 2010

Session I: 15⁰⁰-19⁰⁰

Chairpersons: M. Spirkova and M. Zlatanović

Press Hall

15⁰⁰-15¹⁵ RETENTION OF COLLOIDAL CdS NANOCRYSTALS BY SILICON MOLECULAR FILTER DURING ELECTROPHORESIS

N.S. Filippov^{1,2}, N.V. Vandyшева¹, S.I. Romanov¹, S.S. Kosolobov¹, O.I. Semenova¹, R.O. Anarbaev², D.V. Pyshnyi², I.A. Pyshnaya²

¹*A.V. Rzhanov Institute of Semiconductor Physics of SB RAS, Novosibirsk, Russia,*

²*Institute of Chemical Biology and Fundamental Medicine of SB RAS, Novosibirsk, Russia*

15¹⁵-15³⁰ COMPOSITION, ATOMIC STRUCTURE AND ELECTRONIC PROPERTIES OF FLUORINE PASSIVATED InAs (111)A/ANODIC OXIDE INTERFACE

N.A. Valisheva¹, O.E. Tereshchenko^{1,2}, V.N. Kruchinin¹, S.V. Ereemeev^{3,4}, S.E. Kulkova^{3,4}, A.V. Kalinkin⁵

¹*Novosibirsk Institute of Semiconductor Physics, Novosibirsk, Russia,* ²*Novosibirsk State University, Novosibirsk, Russia,* ³*Institute of Strength Physics and Materials Science, Tomsk, Russia,* ⁴*Tomsk State University, Tomsk, Russia,* ⁵*Boreskov Institute of Catalysis, Novosibirsk, Russia*

15³⁰-15⁴⁵ NEW COMPOSITE CERAMIC MATERIALS FOR PVD TARGETS BASED ON Ti-Al-Si₃N₄-C SYSTEM PRODUCED BY COMBUSTION SYNTHESIS

Yu.S. Pogozhev, E.A. Levashov, D.V. Shtansky, Ph.V. Kiryukhantsev-Korneev
National University of Science and Technology "MISIS", Scientific-Educational Center of SHS, Moscow, Russia

15⁴⁵-16⁰⁰ THE STRUCTURAL ATOMIC MODELS OF W/Si INTERFACES AND PROCESSES OF SELF-ORGANIZATION OF INTERFACE REACTION ZONE IN CVD GROWTH OF TUNGSTEN THIN-FILMS ON SILICON SUBSTRATE

A.V. Andreeva, S.V. Plushcheva

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

- 16⁰⁰-16¹⁵ **SHS METALLURGY OF CAST ALLOYS UNDER HIGH GRAVITY**
V. Sanin, D. Andreev, D. Ikornikov, V. Yukhvid
Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow Region, Russia
- 16¹⁵-16³⁰ **Co-B CATALYSTS FOR HYDROLYSIS OF BORON-BASED COMPLEX HYDRIDES TO GENERATE PURE HYDROGEN FOR PEM FUEL CELL**
V.I. Simagina¹, O.V. Komova¹, A.M. Ozerova¹, O.V. Netskina¹, D.G. Kellerman², G.V. Odegova¹
¹*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*, ²*Institute of Solid State Chemistry UB RAS, Ekaterinburg, Russia*
- 16³⁰-16⁴⁵ **DEVELOPMENT OF NEW TOOL STEELS FOR FORGING DIES**
P. Šuchmann¹, J. Krejčík², P. Fila³, L. Jelen⁴, E. Psík⁵
¹*COMTES FHT, Dobruany, Czech Republic*, ²*SVÚM, Praha, Czech Republic*, ³*ŽDAS, Žďár nad Sázavou, Czech Republic*, ⁴*Vitkovice výzkum a vývoj, Vitkovice, Czech Republic*, ⁵*Kovárna VIVA Zlín, Zlín, Czech Republic*
- 16⁴⁵-17⁰⁰ **INFLUENCE OF CASTING PARAMETERS ON GLASS FORMING ABILITY AND MECHANICAL PROPERTIES OF Zr₄₈Cu₃₆Ag₈Al₈ BULK METALLIC GLASS**
J. Latuch, M. Suligowski, T. Kulik
Warsaw University of Technology, Faculty of Materials Science and Engineering, Warsaw, Poland
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- 17³⁰-17⁴⁵ **THERMAL MEMORY PROPERTIES AND DEPTH INHOMOGENITY OF POLYOLEFINES DETERMINED BY PHOTOACOUSTIC FREQUENCY METHOD**
S. Galović^{1,2}, D.D. Markushev³, M.D. Rabasović³, M. Popović¹, D. Miličević¹, E. Suljovrujić¹, D. Čevizović¹
¹*The "Vinca" Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*, ²*Faculty of Mechanical Engineering Kraljevo, Department of Applied Mechanics, Mathematics and Physics, University of Kragujevac, Kraljevo, Serbia*, ³*Institute of Physics, University of Belgrade, Belgrade-Zemun, Serbia*
- 17⁴⁵-18⁰⁰ **STABLE CRACK GROWTH IN AUTOMOTIVE STEEL SHEETS**
L. Pešek, Ľ Ambriško
Department of Materials Science, Faculty of Metallurgy, Technical University of Kosice, Kosice, Slovakia

- 18⁰⁰-18¹⁵ **CHANGES IN MICROSTRUCTURE OF AIR PLASMA SPRAYED MCrAlY COATINGS AFTER SHORT THERMAL EXPOSURE IN ARGON ATMOSPHERE**
L. Čelko¹, V. Řičánková¹, L. Klakurková¹, E. Dvořáček², T. Podrábský¹, J. Švejcar¹
¹*Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic,* ²*S.A.M. – Metallizing Company, Ltd., Brno, Czech Republic*
- 18¹⁵-18³⁰ **ADSORBATE – INDUCED DIGITAL ETCHING OF GaAs(001) WITH A MONOLAYER PRECISION CONTROLLED BY SURFACE RECONSTRUCTION**
O.E. Tereshchenko^{1,2}, V.L. Alperovich^{1,2}, A.V. Bakulin^{3,4}, S. V. Eremeev^{3,4}, S. E. Kulkova^{3,4}
¹*Institute of Semiconductor Physics, Novosibirsk, Russian Federation,* ²*Novosibirsk State University, Novosibirsk, Russian Federation,* ³*Institute of Strength Physics and Materials Science,* ⁴*Tomsk State University, Tomsk, Russian Federation*
- 18³⁰-18⁴⁵ **OVERALL MODEL OF PLASTICITY AND FAILURE OF METALS**
L.B. Zuev
Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia
- 18⁴⁵-19⁰⁰ **NANO-COATING AS A METHOD TO IMPROVE PHYSICAL AND MECHANIC CHARACTERISTICS OF MATERIALS**
B.S. Semukhin, I.M. Goncharenko, N.N. Koval
Institute of Physics Strain and Material Science, Institute of High Current Electronics Siberian Branch, Russian Academy of Science Tomsk, Russia

SECOND PLENARY SESSION

Tuesday, September 7, 2010

Session II: 09⁰⁰-13³⁰

Chairmen: W. Jaeger, R. Webb and T. Kelly

Conference Hall

09⁰⁰-09³⁰ **ELECTRONICALLY TUNABLE NANOSTRUCTURES**

R. Kruk¹, S. Dasgupta¹, H. Hahn^{1,2}

¹Karlsruhe Institute of Technology (KIT), Institute for Nanotechnology, Karlsruhe, Germany, ²Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt, Darmstadt, Germany

09³⁰-10⁰⁰ **MULTILAYER COATINGS FOR X-RAY OPTICS**

W. Jaeger

Microanalysis of Materials, Institute of Materials Science, Christian-Albrechts-University of Kiel, Kiel, Germany

10⁰⁰-10³⁰ **POLAR OXIDE INTERFACES: STRUCTURE AND COMPOSITION ON THE ATOMIC SCALE**

M. Luysberg

Institute of Solid State Research and Ernst Ruska-Centre, Research Centre Jülich, Germany

10³⁰-11⁰⁰ **QUANTITATIVE NANOMECHANICAL TESTING IN A TEM**

A.M. Minor

Department of Materials Science and Engineering, University of California, Berkeley and National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Break: 11⁰⁰-11³⁰

11³⁰-12⁰⁰ **PRESENT STATUS AND IMPORTANT NEW TRENDS IN ATOM PROBE TOMOGRAPHY**

T.F. Kelly¹, D. Lawrence¹, C. Jones¹, R.M. Ulfing¹, T.J. Prosa¹, D.J. Larson¹

I. Martin², R. Benbalagh², L. Renaud², F. Horr  ard²

¹CAMECA Madison, Madison, WI, USA, ²CAMECA France, Gennevilliers Cedex, France

12⁰⁰-12³⁰ **THE USE OF MeV IONS FOR SECONDARY ION MASS SPECTROMETRY WITH SIMULTANEOUS PIXE AND RBS**

B. Jones, V. Palitsin, M.J. Bailey, A.A. Karim, J. Mody, R. Webb
Surrey Ion Beam Centre, University of Surrey, Guildford, Surrey, United Kingdom

12³⁰-13⁰⁰ **FIRST-PRINCIPLES STUDIES ON TRADITIONAL AND EMERGING MATERIALS**

L. Tsetseris^{1,2}
¹*Department of Physics, National Technical University of Athens, Greece,*
²*Department of Physics and Astronomy, Vanderbilt University, USA*

13⁰⁰-13³⁰ **MECHANISMS OF DYNAMIC VOID GROWTH BY DISLOCATION EMISSION FOR NANO AND MICRON SIZE VOIDS**

V.A. Lubarda
Montenegrin Academy of Sciences and Arts, Podgorica, Montenegro, & Department of Mechanical and Aerospace Engineering, UCSD, La Jolla, CA, USA

Break: 13³⁰-15⁰⁰

SYMPOSIUM C: NANOSTRUCTURED MATERIALS

Session I: 15⁰⁰-19⁰⁰

Chairmen: J. Nedeljković and M. Damnjanović

Conference Hall

- 15⁰⁰-15¹⁵ **CHARACTERIZATION OF INTERFACES IN A MODEL CERAMIC-METAL SYSTEM**
M.K. Santala¹, V.R.Radmilovic², R.Giulian³, M.C. Ridgway³, R. Gronsky⁴, A.M. Glaeser⁴
¹*Condensed Matter & Materials Division, Lawrence Livermore National Laboratory, CA, USA,* ²*National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA, USA,* ³*Department of Electronic Materials Engineering, Australian National University, Canberra, ACT, Australia,* ⁴*Department of Materials Science & Engineering, University of California, Berkeley, CA, USA*
- 15¹⁵-15³⁰ **SYNTHESIS OF ZnO-C NANOCOMPOSITE USING FUSED SALT ELECTROLYSIS**
A.R. Kamali, D.J. Fray
Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, U.K.
- 15³⁰-15⁴⁵ **STRUCTURAL AND LUMINESCENCE STUDY OF In AND Fe DOPED ZnO NANOWIRES AND NANORIBBONS**
B. Alemán, P. Fernández, J. Piqueras
Dpt.Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Madrid, Spain
- 15⁴⁵-16⁰⁰ **MICROSTRUCTURE AND CATALYTIC PROPERTIES OF OXIDE THIN FILMS DEPOSITED BY PLD TECHNIQUE**
J. Kusinski¹, A. Kopia¹, M. Chmielowska¹, J.R. Gavarrí²
¹*University of Science and Technology, AGH, Cracow, Poland,* ²*Université du Sud Toulon Var, IM2NP, UMR CNRS 6242, BP 20132, La Garde Cedex, France*
- 16⁰⁰-16¹⁵ **DIFFRACTION FROM MS2 NANOTUBES**
M. Damnjanović, I. Milošević
University of Belgrade, Faculty of Physics, NanoLab, Belgrade, Serbia
- 16¹⁵-16³⁰ **COILED SINGLE-WALL CARBON NANOTUBES**
I. Milošević, M. Damnjanović
University of Belgrade, Faculty of Physics, NanoLab, Belgrade, Serbia

- 16³⁰-16⁴⁵ **INTER-LANDAU LEVEL SCATTERING PROCESSES IN MAGNETIC FIELD ASSISTED THz QUANTUM CASCADE LASER**
J. Radovanović², A. Daničić², V. Milanović¹, D. Indjin³, Z. Ikonić³
¹*School of Electrical Engineering, University of Belgrade, Belgrade, Serbia,* ²*Vinča Institute of Nuclear Sciences, Belgrade, Serbia,* ³*Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds, UK*
- 16⁴⁵-17⁰⁰ **INFLUENCE OF THE NANOSTRUCTURE ON THE SURFACE AND BULK PHYSICAL PROPERTIES OF MATERIALS**
N.V. Kamanina^{1,2}, N.A. Shurpo¹, P.Ya. Vasilyev¹, V.I. Studeonov¹, D.P. Uskokovic³
¹*Vavilov State Optical Institute, St. Petersburg, Russia,* ²*Electrotechnical University ("LETI"), St. Petersburg, Russia,* ³*Institute of Technical Sciences of the SASA, Belgrade, Serbia*
- Break: 17⁰⁰-17³⁰**
- 17³⁰-17⁴⁵ **ALUMINOPHOSPHATE-BASED CHABAZITE AS A NANO-OXIDE CARRIER**
N. Rajić¹, A. Rečnik²
¹*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,* ²*Jožef Štefan Institute, Ljubljana, Slovenia*
- 17⁴⁵-18⁰⁰ **NOVEL POLYCARBONATE-BASED POLYURETHANE ELASTOMERS, PREPARATION AND CHARACTERIZATION**
M. Špírková¹, R.Poreba¹, A. Strachota¹, J. Pavličević², J. Budinski-Simendić²
¹*Institute of Macromolecular Chemistry ASCR, v.v.i. (IMC), Prague, Czech Republic,* ²*Faculty of Technology, Novi Sad, Serbia*
- 18⁰⁰-18¹⁵ **LASER ELECTRODISPERSION FABRICATION OF NANOPATTERNS FOR SER(R)S OPERANDO SPECTROSCOPY**
V. Sans¹, V. Kozhevin^{2,3}, D. Yavsin^{2,3}, I. Kuzmin², S. Gurevich^{2,3}, A. Lapkin¹
¹*School of Engineering, University of Warwick, United Kingdom,* ²*INCATTECH LLC, St. Petersburg, Russia,* ³*Ioffe Physical Technical Institute, Russian Academy of Sciences, Russia*

- 18¹⁵-18³⁰ **SYNTHESIS OF MESOPOROUS TITANIA FILMS TEMPLATED BY NOVEL AMPHIPHILIC TRIBLOCK COPOLYMER PEO-PB-PEO**
E. Ortel¹, L. Chuenchom^{1,2}, B. Smarsly², R. Kraehnert^{1,*}
¹*Technical University of Berlin, Department of Chemistry, Berlin, Germany,*
²*Justus-Liebig-Universität Gießen, Physikalisch-Chemisches Institut, Gießen, Germany*
- 18³⁰-18⁴⁵ **CHARGE MEMORY EFFECTS IN InN NANODOTS**
E. Sarantopoulou, Z. Kollia, A.C. Cefalas
National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Athens, Greece
- 18⁴⁵-19⁰⁰ **NANOSIZE WO₃ FOR GAS SENSING AND PHOTOCATALYSIS**
B. Fórizs¹, I.M. Szilágyi², O. Rosseler³, J. Mizsei⁴, G. Tárkányi⁵, P. Király⁴, P. Németh⁴, K. Vargáné Josepovits¹, B. Vajna¹, A. Tóth⁵, Á. Szegedi⁴
¹*Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Hungary,* ²*Materials Structure and Modeling Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, Hungary,* ³*LMSPC, Strasbourg, French,* ⁴*Department of Electron Devices, Budapest University of Technology and Economics, Hungary,* ⁵*Chemical Research Center, Institute of Structural Chemistry, Hungarian Academy of Sciences, Budapest, Hungary*

SYMPOSIUM D: COMPOSITES

Tuesday, September 7, 2010

Session I: 15⁰⁰-19⁰⁰

Chairpersons: D. Nedelcu and S. Bošković

Press Hall

- 15⁰⁰-15¹⁵ **SOME ASPECTS OF PROCESSING AND PROPERTIES OF COMPOSITE MATERIAL WITH Si-C PARTICLES**
D. Nedelcu¹, I. Carcea², L. Tabacaru¹, C. Ciofu¹
¹"Gheorghe Asachi" Technical University of Iasi-Romania, Department of Machine Manufacturing Technology, Iasi, Romania, ²"Gheorghe Asachi" Technical University of Iasi-Romania, Department of Materials Processing Technologies and Equipments, Iasi, Romania
- 15¹⁵-15³⁰ **MICROSTRUCTURE –MECHANICAL PROPERTIES RELATIONS IN PRESURELESS SINTERED SiC-TiB₂ COMPOSITE**
D. Bučevac¹, B. Matović¹, S. Zec¹, S. Bošković¹, V. Krstić²
¹Institute of Nuclear Sciences Vinča, University of Belgrade, Belgrade, Serbia, ²Department of Mechanical and Materials Engineering, Queen's University, Kingston, Ontario, Canada
- 15³⁰-15⁴⁵ **STUDY OF FORMATION AND MESOSTRUCTURE OF YTTRIUM HYDROXOCARBONATE MONODISPERSE SPHERICAL PARTICLES**
A.S. Vanetsev¹, A.E. Barantchikov¹, G.P. Kopitsa², I.G. Chuvashova¹, A.S. Shaporev¹, V. Haramus³
¹Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia, ²Petersburg Nuclear Physics Institute RAS, Gatchina, Russia, ³GKSS Research Centre, Geesthacht, Germany
- 15⁴⁵-16⁰⁰ **METAL-MATRIX COMPOSITES DISPERSION-STRENGTHENED BY NANOPARTICLES FOR DIAMOND TOOLS APPLICATION**
A. Zaitsev¹, E. Levashov¹, V. Kurbatkina¹, S. Rupasov¹, D. Sidorenko¹, V. Andreev²
¹National University of Science and Technology "MISIS", Moscow, Russia, ²Company "Kermet" Ltd., Moscow, Russia
- 16⁰⁰-16¹⁵ **TRIBOLOGICAL PROPERTIES OF Si₃N₄ + SiC AND Al₂O₃ + SiC NANOCOMPOSITES**
J. Dusza
Institute of Materials Research, SAS, Kosice, Slovakia

- 16¹⁵-16³⁰ **PROCESSING TECHNOLOGIES FOR DISCONTINUOUSLY REINFORCED LIGHT METALS**
M. Wenzelburger, R. Gadow
Universität Stuttgart, Institut für Fertigungstechnologie keramischer Bauteile (IFKB), (Institute for Manufacturing Technologies of Ceramic Components and Composites), Stuttgart, Germany
- 16³⁰-16⁴⁵ **MANUFACTURING OF CONTINUOUS FIBER REINFORCED LIGHT METAL MATRIX COMPOSITES BY THERMAL SPRAYING OF PREPREGS**
M. Silber, R. Gadow
Institute for Manufacturing Technologies of Ceramic Components and Composites, University of Stuttgart, Stuttgart, Germany
- 16⁴⁵-17⁰⁰ **LOCK-IN IR THERMOGRAPHY METHOD FOR EVALUATION OF LIGHT COMPOSITE ARMOURS**
W. Swiderski¹, M. Szudrowicz²
¹Military Institute of Armament Technology, Zielonka, Poland, ²Military Institute of Armour & Automotive Technology, Sulejowek, Poland
- Break: 17⁰⁰-17³⁰**
- 17³⁰-17⁴⁵ **SPIN-DEPENDENT MAGNETORESISTANCE AND MAGNETIZATION IN OXIDIZED FeCoZr-AL₂O₃ GRANULAR NANOCOMPOSITES WITH «CORE-SHELL» STRUCTURE**
J. Fedotova¹, J. Kasiuk¹, J. Przewoznik², C. Kapusta², J. Zukrowski²
¹National Centre for High Energy and Particle Physics, Belarusian State University, Minsk, Belarus, ²Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Cracow, Poland
- 17⁴⁵-18⁰⁰ **NANOCOMPOSITE MATERIALS BASED ON FLUORITE OXIDES AND Ni/YSZ: SYNTHESIS, PROPERTIES AND CATALYTIC PERFORMANCE IN STEAM REFORMING OF CH₄ AND BIOFUELS**
N. Mezentseva¹, G. Alikina¹, R. Bunina¹, J.R.H. Ross², V. Sadykov¹
¹Boriskov Institute of Catalysis, Novosibirsk Russia, ²Centre of Environmental Research, University of Limerick, Limerick, Ireland
- 18⁰⁰-18¹⁵ **A STUDY ON DELAMINATION-FREE DRILLING OF CARBON FIBRE REINFORCED PLASTICS**
C.M. Machado, J. Pamies Teixeira
UNIDEMI, Departamento de Engenharia Mecânica e Industrial, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal

- 18¹⁵-18³⁰ **PREPARATION AND OPTIMALIZATION OF SILICON OXYCARBIDE COMPOSITES TOUGHENED BY INORGANIC FIBERS BY PYROLYSIS OF PRECURSOR COMPOSITES WITH SILOXANE MATRIX**
A. Strachota¹, M. Černý², P. Glogar², Z. Sucharda², Z. Chlup³, I. Dlouhý³, V. Kozák³
¹Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, v.v.i., Praha, Czech Republic, ²Institute of Rock Structure and Mechanics, Academy of Sciences of the Czech Republic, v.v.i., Praha, Czech Republic, ³Institute of Physics of Materials of the Academy of Sciences of the Czech Republic, v.v.i., Brno, Czech Republic
- 18³⁰-18⁴⁵ **PHASE RELATIONS AND ADVANCED MATERIALS IN THE CeO₂-Ln₂O₃ SYSTEMS**
E.R. Andrievskaya, O.A. Kornienko, A.V. Sameljuk
Institute of Materials Science Problems, National Ukrainian Academy of Sciences, Kiev, Ukraine
- 18⁴⁵-19⁰⁰ **PROCESSING OF INTEGRAL SKIN CELLULAR POLYMERIC COMPOSITES IN RAPID ROTATIONAL FOAM MOLDING**
R. Pop-Iliev
Faculty of Engineering and Applied Science, University of Ontario Institute of Technology, Oshawa, Ontario, Canada

THIRD PLENARY SESSION

Wednesday, September 8, 2010

Session III: 09⁰⁰-13⁰⁰

Chairmen: R. Ritchie, D. Raković and M. Senna

09⁰⁰-09³⁰ **CROSS-LINKING BEHAVIOR IN GELATIN – HYDROXYAPATITE NANOCOMPOSITE**

Y. Shirakura, M. Senna

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

09³⁰-10⁰⁰ **MIMICKING THE GENESIS OF TOOTH ENAMEL**

V. Uskoković, S. Habelitz

Division of Biomaterials and Bioengineering, University of California, San Francisco, CA, USA

10⁰⁰-10³⁰ **ELECTRON ENERGY-LOSS SPECTROSCOPY (EELS) FOR NANOPLASMONIC APPLICATIONS IN MATERIALS SCIENCE**

A.L. Koh

Department of Materials, Imperial College London, London, UK

10³⁰-11⁰⁰ **TAILORED IMPLANTS BY SELECTIVE ELECTRON BEAM MELTING**

C. Körner, P. Heinl

Universität Erlangen-Nürnberg, Lehrstuhl Werkstoffkunde und Technologie der Metalle WTM, Erlangen, Germany

Break: 11⁰⁰-11³⁰

11³⁰-12⁰⁰ **PLASMA TAILORED NANOSTRUCTURES AND THEIR ADVANCED APPLICATIONS**

U. Cvelbar

Plasma lab F4, Jozef Stefan Institute, Ljubljana, Slovenia

12⁰⁰-12³⁰ **NOVEL MECHANOCHEMICAL SYNTHESIS OF CARBON NANOMATERIALS BY A HIGH-SPEED BALL-MILLING PROCESS**

S. Ohara, Z. Tan, K. Sato, H. Abe

Joining and Welding Research Institute, Osaka University, Ibaraki, Osaka, Japan

12³⁰-13⁰⁰ **NT-MDT.Co PRESENTATION**

I. Bykov

NT-MDT.Co

FORTH PLENARY SESSION

Thursday, September 9, 2010

Session IV: 09⁰⁰-12³⁰

Chairmen: D. Suvorov, S. Milonjić and A. Labarta

09⁰⁰-09³⁰ **FROM HIGH TO LOW PERMITTIVITY GLASS-FREE MATERIALS FOR LTCC TECHNOLOGY**

D. Suvorov, M. Maček Kržmanc

Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia

09³⁰-10⁰⁰ **RECENT ADVANCES IN MAGNETIC NANOSTRUCTURES**

A. Labarta, N. Pérez, M. Kovylyina, M. García del Muro, O. Iglesias, X. Batlle

Departament de Física Fonamental and Institut de Nanociència i Nanotecnologia (IN2UB), Universitat de Barcelona, Barcelona, Spain

10⁰⁰-10³⁰ **CHARACTERIZATION OF MAGNETIC NANOCRYSTALS FORMED BY MAGNETOTACTIC BACTERIA**

M. Pósfai¹, T. Kasama², R E. Dunin-Borkowski²

¹Department of Earth and Environmental Sciences, University of Pannonia, Veszprém, Hungary, ²Center for Electron Nanoscopy, Technical University of Denmark, Kongens Lyngby, Denmark

10³⁰-11⁰⁰ **BONDED INTERMETALLIC POWDERS FOR THE APPLICATION IN MAGNETIC REFRIGERATION**

B. Podmiljšak, P.J. McGuinness, M. Soderžnik, S. Kobe

Jožef Stefan Institute, Ljubljana, Slovenia

Break: 11⁰⁰-11³⁰

11³⁰-12⁰⁰ **CRYSTAL STRUCTURE OF APATITE TYPE RARE-EARTH SILICATE SrLn₄Si₃O₁₃**

R. Ubić, D. Leu, S. Thomas, M. Sebastian

Boise State University, Boise, Idaho, USA, National Institute for Interdisciplinary Science and Technology, Trivandrum, India

12⁰⁰-12³⁰ **HYDROTHERMAL SYNTHESIS AND POST HEAT-TREATMENT OF (K,Na)NbO₃ PARTICLES**

J.-Ho. Jeon, B.-J. Shin, S.-Y. Choi, J.-B. Lim,

Korea Institute of Materials Science, Changwon, Korea

SYMPOSIUM E: BIOMATERIALS

Friday, September 4, 2009

Session I: 09⁰⁰-11³⁰

Chairmen: Dj. Koruga and N. Ignjatović

09⁰⁰-09¹⁵ HIGH-VELOCITY SUSPENSION FLAME SPRAYED (HVSFS) BIOACTIVE HYDROXYAPATITE COATINGS

N. Stiegler, A. Killinger, R. Gadow

Institute for Manufacturing Technologies of Ceramic Components and Composites (IMTCCC), University of Stuttgart, Stuttgart, Germany

09¹⁵-09³⁰ NANO-BIORESORBABLE POLYMER SPHERES AS CARRIERS FOR TRANSDERMAL DELIVERY OF KETOPROFENE

N. Ignjatović¹, S. Vučen², G. Vuleta³, D. Uskoković¹

¹Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, ²Faculty of Medicine, Department of Pharmacy, University of Banja Luka, Bosnia and Herzegovina, ³Department of the Pharmaceutical Technology and Cosmetology, Faculty of Pharmacy, University of Belgrade, Serbia

09³⁰-09⁴⁵ PLGA NANOSPHERES AS DRUG CARRIERS FOR WATER- SOLUBLE VITAMINS: IN VITRO AND IN VIVO STUDIES

M. Stevanović¹, T. Maksin², J. Petković³, M. Filipič³, D. Uskoković¹

¹Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, ²The Institute of Nuclear Sciences "Vinča", Belgrade, Serbia, ³National Institute of Biology, Ljubljana, Slovenia

09⁴⁵-10⁰⁰ SONOCHEMICAL SYNTHESIS OF SILVER NANOPARTICLES AND SILVER/HYDROXYAPATITE NANOCOMPOSITES

M. Vukomanović^{1,2}, I. Bračko¹, S.D. Škapin¹, D. Suvorov¹, D. Uskoković²

¹Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia, ²Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia

10⁰⁰-10¹⁵ THE INVESTIGATION OF PERIODONTAL LIGAMENT CELL GROWTH ONTO WATER/O₂ PLASMA TREATED PCL SUBSTRATES

H.T. Şaşmazel¹, S. Manolache², M. Gümüşderelioglu³

¹Atılım University, Department of Materials Engineering, Incek, Gölbaşı, Ankara, Turkey, ²Wisconsin/Madison University, Center for Plasma-Aided Manufacturing Unit (CPAM), Wisconsin, USA, ³Hacettepe University, Chemical Engineering and Bioengineering Departments, Beytepe, Ankara, Turkey

10¹⁵-10³⁰ **EPIDERMAL LAYERS CHARACTERISATION BY OPTO-MAGNETIC FINGERPRINT**

Dj. Koruga¹, J. Bandić³, G. Janjić¹, Č. Lalović¹, D. Dobrosavljević Vukojević²
¹NanoLab, Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia, ²Institute of Dermatovenerology, School of Medicine University of Belgrade, Belgrade, Serbia, ³ORS Hospital, Belgrade, Serbia

Break: 10³⁰-11⁰⁰

11⁰⁰-11¹⁵ **HYDROPHOBIC-HYDROPHILIC INTERACTIONS IN PROTEIN FOLDING, PROTEIN-PROTEIN ASSOCIATION AND MOLECULAR RECOGNITION**

A. Ben-Naim

Department of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

11¹⁵-11³⁰ **LIQUID CRYSTALLINE WATER AND THE LIVING STATE**

M.-W. Ho

Institute of Science in Society, London, UK

11³⁰-12⁰⁰ **CLOSING CEREMONY**

POSTER SESSION I

Tuesday, September 7, 2010, 20³⁰-22⁰⁰

SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

P.S.A.1. ALUMINIDE FORMATION BY SPARK ALLOYING OF METALLIC SUBSTRATE

M. Torkar, M. Godec, B. Šuštaršič, M. Jenko
Institute of Metals and Technology, Ljubljana, Slovenia

P.S.A.2. PREPARATION AND CHARACTERISATION OF MAGHEMITE-CM-DEXTRAN FERROFLUID FOR THE APPLICATION IN MAGNETIC HYPERTHERMIA

G. Ferik¹, M. Bekovič², D. Makovec³, M. Drofènik^{1,3}
¹*University of Maribor, Faculty of Chemistry and Chemical Engineering, Maribor, Slovenia,* ²*University of Maribor, Faculty of Electrical Engineering and Computer Science, Maribor, Slovenia,* ³*Department of Material Synthesis, Jožef Stefan Institute, Ljubljana, Slovenia*

P.S.A.3. SYNTHESIS OF COPPER-NICKEL NANOPARTICLES PREPARED BY MECHANICAL MILLING OR MICROEMULSION METHOD

I. Ban¹, J. Damiš¹, M. Drofènik^{1,2}, D. Makovec²
¹*University of Maribor, Faculty of Chemistry and Chemical Engineering, Maribor, Slovenia,* ²*Jožef Stefan Institute, Ljubljana, Slovenia*

P.S.A.4. SYNTHESIS AND CHARACTERIZATION OF Cu-Ni MAGNETIC NANOPARTICLES FOR HYPERTHERMIA APPLICATIONS

J. Damiš¹, I. Ban¹, M. Drofènik^{1,2}, D. Makovec²
¹*University of Maribor, Faculty of Chemistry and Chemical Engineering, Maribor, Slovenia,* ²*Jožef Stefan Institute, Ljubljana, Slovenia*

P.S.A.5. DEPENDENCE OF SURFACE AND ZETA POTENTIALS OF SILICA ON pH IN AQUEOUS ELECTROLYTE SOLUTIONS

S.K. Milonjić
The Vinča Institute of Nuclear Sciences, Belgrade, Serbia

- P.S.A.6. **NON-ISOTHERMAL THERMOGRAVIMETRIC STUDY OF CuO REDUCTION BY HYDROGEN**
D. Jelić¹, S. Mentus², M. Mališić³
¹Medicine Faculty, Pharmacy Department, University of Banja Luka, Bosnia and Herzegovina, ²Faculty of Physical Chemistry, University of Belgrade, Serbia, ³Public Educational Institution, Herceg Novi, Montenegro
- P.S.A.7. **MICROEMULSION-MEDIATED HYDROTHERMAL SYNTHESIS OF LiFePO₄ CATHODE MATERIAL**
M. Jović¹, D. Jugović¹, M. Mitrić², N. Cvjetičanin³, D. Uskoković¹
¹Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, ²The Vinca Institute, Condensed Matter Physics Laboratory, Belgrade, Serbia, ³Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia
- P.S.A.8. **SAMARIUM-DOPED CERIA THIN FILMS ON FTO GLASS OBTAINED BY ELECTRODEPOSITION**
Lj.S. Živković^{1,2}, V. Lair¹, O. Lupan^{1,3}, M. Cassir¹, A. Ringuedé¹
¹Laboratoire d'Electrochimie, Chimie des Interfaces et Modélisation pour l'Energie, UMR 7575 CNRS- ENSCP - Chimie-Paristech, Paris, France, ²Vinča Institute of Nuclear Sciences, Serbia, ³Technical University of Moldova, Chisinau, Republic of Moldova
- P.S.A.9. **NANOCOMPOSITES Y₂O₃:RE@SiO₂ AND Gd₂O₃:RE@SiO₂: MICROWAVE SYNTHESIS AND LUMINESCENT PROPERTIES**
A.S. Vanetsev¹, E.A. Karpukhina¹, A.E. Barantchikov¹, Yu.V. Orlovskii², V.V. Osiko², O.M. Gaitko¹, I.G. Chuvashova¹
¹Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia, ²Prokhorov General Physics Institute RAS, Moscow, Russia
- P.S.A.10. **PARTICLES FORMATION DURING PULSE PLASMA NITRIDING AND a-CN_x:H COATING DEPOSITION ON HOT WORK STEEL SAMPLES**
M. Zlatanović¹, N. Popović²
¹School of Electrical Engineering, Beograd, Serbia, ²Institute of Nuclear Sciences Vinča, Beograd, Serbia
- P.S.A.11. **THE INFLUENCE OF CHEMICAL TREATMENT OF CARBON MONOLITH ON SILVER DEPOSITION**
M. Vukčević¹, A. Kalijadis², Z. Jovanović², Z. Laušević², M. Laušević¹
¹Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia
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- P.S.A.12. **SURFACE COMPLEXES FORMATION ON BORON IRRADIATED AND BORON DOPED GLASSY CARBON**
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A.P. Malygin, D.V. Alexandrov, I.V. Alexandrova
Ural State University, Ekaterinburg, Russia
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L. Cieniek
AGH – University of Science and Technology, Krakow, Poland
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S. Kac
AGH-University of Science and Technology, Faculty of Metals Engineering and Computer Industrial Science, Krakow, Poland
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D. Peruško¹, M. Milosavljević¹, S. Petrović¹, M. Mitrić¹, V. Milinović¹, C. Jeynes², P. Panjan³
¹Vinča Institute of Nuclear Sciences, Belgrade, Serbia, ²University of Surrey, Ion Beam Centre, Guildford, UK, ³Jožef Stefan Institute, Ljubljana, Slovenia
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S. Dimitrijević¹, V. Trujić¹, M. Rajčić Vujasinović²
¹Institute of Mining and Metallurgy Bor, Serbia, ²Technical Faculty Bor, University of Belgrade, Bor, Serbia
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Z. Baroš¹, B. Adnadjević²
¹Higher Education School of Professional Studies - Belgrade Polytechnic, Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

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M.L. Busurina, S.M. Busurin, M.V. Kuznetsov
Institute of Structural Macrokinetics and Materials Science RAS, Chernogolovka, Moscow region, Russia
- P.S.A.20. **INFLUENCE OF TPA⁺ CONTENT ON SILICALITE-1 CRYSTALLIZATION**
O.A. Kovačević¹, B.T. Kovačević¹, D. Arandjelović¹, L.L. Pezo¹, V. Dondur², Ž.Lj. Tešić³
¹*Institute of General and Physical Chemistry, Belgrade, Serbia*, ²*Faculty of Physical Chemistry, Belgrade, Serbia*, ³*Faculty of Chemistry, Belgrade, Serbia*
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O.A. Kovačević¹, B.T. Kovačević¹, D. Arandjelović¹, L.L. Pezo¹, V. Dondur², Ž.Lj. Tešić³
¹*Institute of General and Physical Chemistry, Belgrade, Serbia*, ²*Faculty of Physical Chemistry, Belgrade, Serbia*, ³*Faculty of Chemistry, Belgrade, Serbia*
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N. Številová¹, I. Filkova¹, K. Baltakys²
¹*Technical University of Kosice, Civil Engineering Faculty, Institute of Building and Environmental Engineering, Kosice, Slovak Republic*, ²*Kaunas University of Technology, Faculty of Chemical Technology, Department of Silicate Technology, Kaunas, Lithuania*
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I. Stojković¹, N. Cvjetičanin¹, S. Mentus^{1*}
¹*University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia*, ^{*}*Serbian Academy of Science and Arts, Belgrade, Serbia*
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B. Holló¹, V.M. Leovac¹, V. Divjaković¹, Z. Tomić², K. Mészáros Szécsényi¹
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D. Radanović¹, A. Bacchi², G. Pelizzi², T. Todorović³, K. Andjelković³
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K. Andjelković¹, G. Bogdanović², D. Jovanović³, D. Mitić¹, Dj. Miodragović¹
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M. Jovičić, R. Radičević
University of Novi Sad, Faculty of Technology, Novi Sad, Serbia
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J. Budinski-Simendić¹, N. Vukić¹, M. Špirkova², J. Pavličević¹, I. Krakovsky³, R. Radičević¹, K. Dušek²
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M.T. Šumar Ristović¹, K.K. Andjelković¹, D. Minić², D. Poletić³, Dj.U. Miodragović¹, Z. Miodragović¹
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A.M. Hatab¹, F.B. Abudaia², H.A. Saadawi³, M.E.M. Zorgani⁴
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V. Jašo, D. Stoiljković, R. Radičević
Faculty of Technology, University of Novi Sad, Novi Sad, Serbia
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E.T. Pecev, Z.M. Grahovac, S.S. Mitić, A.N. Pavlović
Faculty of Natural Sciences and Mathematics, Department of Chemistry, Niš, Serbia
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Lj. Veselinović¹, M. Mitrić², S. Marković¹, D. Uskoković¹
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Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia

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A. Stanković¹, Z. Stojanović¹, S. Škapin², I. Bračko², D. Uskoković¹
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Z. Stojanović, Lj. Veselinović, S. Marković, D. Uskoković
Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia
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I. Dugandžić¹, V. Lojpur¹, L. Mančić¹, M.E. Rabanal², O. Milošević¹
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Z.Ž. Lazarević¹, Č. Jovalekić², M.J. Romčević¹, M.B. Pavlović², N.Ž. Romčević¹
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- P.S.A.41. **ELOUTION RATE OF MONOMERS FROM RESIN-BASED COMPOSITES CURRED WITH A HALOGEN LIGHT-CURING UNIT**
D. Manojlović¹, M. Radišić², T. Vasiljević², S. Živković¹, M. Laušević², V. Miletić¹
¹*University of Belgrade, School of Dentistry, Department of Restorative Dentistry and Endodontics, Belgrade, Serbia*, ²*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia*
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Z. Vosika¹, Z. Mitrović¹, J. Bandić², J. Simić-Krstić¹, M. Lazarević¹, Dj. Koruga¹
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R. Rudolf^{1,2}, M. Brunčko^{1,3}, K. Mehrabi³, A.C. Kneissl³, M. Čolić⁴, N. Romčević⁵, I. Anžel¹
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N. Mitrović¹, M. Milošević¹, K. Čolić¹, I. Hut¹, I. Tanasić², A. Petrović³, A. Sedmak³
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K. Čolić¹, A. Sedmak², I. Hut¹
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D. Manojlović¹, V. Miletić¹, M. Milošević², N. Mitrović², E. Džindo², A. Sedmak³
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I.S. Ristić¹, J.K. Budinski-Simendić¹, S.M. Cakić², M. Špirkova³, A. Strachota³, I. Krakovsky⁴
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B. Čolović, V.Jokanović
Institute of Nuclear Sciences "Vinča", Laboratory of Radiation Chemistry and Physics, Belgrade, Serbia
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A. Kalezić-Glišović, A. Maričić, R. Simeunović, S. Randjić
Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems, Technical Faculty Čačak, Čačak, Serbia
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O. Pešić¹, B. Jordović¹, A. Maričić¹, J. Stevanović², S. Djukić²
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- P.S.A.52. **THE EFFECT OF CHANGE IN ELECTRON STATE DENSITY AT FERMI LEVEL DURING THE MECHANICAL STRAIN ON SENSITIVITY COEFFICIENT OF THE RIBBON-SHAPED AMORPHOUS ALLOY $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$ AS FORCE SENSOR**
A. Maričić, M. Spasojević, A. Kalezić-Glišović, N. Mitrović, L. Ribić-Zelenović
Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Alloys, Technical Faculty Čačak, Čačak, Serbia
- P.S.A.53. **CORRELATION BETWEEN HYDROGEN PRESSURE CHANGE AND RESISTIVITY CHANGE DURING HYDROGEN ABSORPTION ON NON PALLADIUM-COATED AND PALLADIUM-COATED COBALT POWDER**
D.M. Minić, A. Kalezić-Glišović, M. Spasojević, A.M. Maričić
Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Alloys, Technical Faculty Čačak, Čačak, Serbia
- P.S.A.54. **MICROSTRUCTURAL AND MAGNETIC PROPERTIES OF ELECTROCHEMICALLY DEPOSITED $\text{Ni}_x\text{Fe}_y\text{W}_z$ ALLOY**
N. Mitrović¹, M. Spasojević², L. Ribić-Zelenović², A. Maričić¹
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T. Barudžija¹, V. Kusigerski¹, N. Cvjetičanin², V. Spasojević¹, M. Mitrić¹
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V. Djordjević, M. Nikolić, Ž. Antić, M. Mitrić, M.D. Dramićanin
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

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M. Nikolić, V. Djordjević, Ž. Antić, R. Krsmanović, M.D. Dramićanin
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

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Z.Ž. Lazarević, N.Ž. Romčević, M.J. Romčević, S. Kostić
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Ecomaterials and Renewable Energy Research Center (ERERC), Nanjing University, Nanjing, China

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N. Ivanović¹, I. Radisavljević¹, N. Novaković¹, M. Manasijević¹, D. Colognesi²
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- P.S.B.7. **5 NM STRUCTURES PRODUCED BY DIRECT LASER WRITING**
S. Jinga¹, E. Pavel², E. Andronescu¹, C. Jinga¹, B.S. Vasile¹
¹*Department of Science and Engineering of Oxide Materials, Faculty of Applied Chemistry and Materials Science, University "Politehnica" of Bucharest, Bucharest, Romania,* ²*Storex Technologies, Bucharest, Romania*
- P.S.B.8. **SYNTHESIS AND CHARACTERIZATION OF PURE AND DOPED Ba(Mg_{1/3}Ta_{2/3})O₃ NANOPOWDERS**
C. Jinga¹, E. Andronescu¹, C. Jinga¹, C. Matei¹, D. Berger¹, S. Jinga¹, A. Ioachim²
¹*University "Politehnica" of Bucharest, Bucharest, Romania,* ²*National Institute of Materials Physics, Bucharest-Magurele, Romania*
- P.S.B.9. **ROOM-TEMPERATURE FERROMAGNETISM IN Zn-Mn-O, X-RAY PHOTOEMISSION SURFACE STUDY**
D. Milivojević¹, B. Babić-Stojić¹, J. Blanuša¹, J. Kováč²
¹*Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia,* ²*Jožef Stefan Institute, Ljubljana, Slovenia*
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D. Milivojević¹, B. Babić-Stojić¹, V. Jokanović¹, Z. Jagličić², D. Makovec³
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- P.S.B.11. **SEGMENTED THERMISTORS PRINTED USING NTC NANOMETRIC PASTE ON ALUMINA AND Sr-FERRITE SUBSTRATES**
T. Ivetić¹, B. Radojčić², M.V. Nikolić³, M. Luković², O. Aleksić³
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- P.S.B.12. **THE INFLUENCE OF THE ATMOSPHERE AND IMPULSE EFFECT OF EXTERNAL MAGNETIC FIELD ON THE MAGNETIC FEATURES OF MnZn-FERRITE DURING THE PROCESS OF SINTERING**
Z. Ristanović¹, M. Plazinić², D. Sretenović¹, J. Živanić²
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- P.S.B.13. THE INFLUENCE OF THE PORE GEOMETRY ON THE MECHANICAL PROPERTIES OF POROUS HAP-BASED BIOCERAMICS**
Dj. Veljović¹, I. Balać², S. Putić¹, R. Jančić-Hajneman¹, B. Jokić¹, R. Petrović¹, Dj. Janačković¹
¹Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,
²Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia
- P.S.B.14. HIGH TEMPERATURE OPTICAL SPECTROSCOPY OF REDUCED AND N-DOPED TiO₂**
J. Shi¹, J. Saatz¹, B. Bauer¹, D.-K. Lee², M. Senna¹, K.D. Becker¹
¹Institute of Physical and Theoretical Chemistry, Technische Universität Braunschweig, Braunschweig, Germany, ²Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany
- P.S.B.15. LOW TEMPERATURE MAGNETIC PROPERTIES OF Pr_{0.7}(Ca,Sr)_{0.3}CoO₃ OXIDES**
I.G. Deac, A. Vladescu, I. Balasz, A. Tunyagi, R. Tetean
Babes-Bolyai University Cluj-Napoca, Faculty of Physics, Cluj-Napoca, Romania
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B. Gligorijević¹, H. Schmidt², M. Šćepanović³, M. Kutin¹, M. Davidović¹
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¹Vinča Institute of Nuclear Sciences, Belgrade, Serbia, ²Institute for Multidisciplinary Research, Belgrade, Serbia
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¹Institute of Nuclear Sciences „Vinča“, Belgrade, Serbia, ²Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

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¹*Institute of Physics, Belgrade, Serbia,* ²*Institute of Physics PAS, Warsaw, Poland,* ³*Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, Russia*
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¹*Institute of Techniques, University of Pedagogy, Krakow, Poland,* ²*Institute of Technical Sciences of SASA, Belgrade, Serbia,* ³*Lviv National University by Ivan Franko, Lviv, Ukraine,* ⁴*University of Forestry and Wood Technology, Lviv, Ukraine*
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¹*Institute of Technical Sciences of SASA, Belgrade, Serbia,* ²*Faculty for Agriculture, University of Belgrade, Belgrade, Serbia,* ³*Faculty for Electronics, University of Niš, Niš, Serbia,* ⁴*The Vinča Institute of Nuclear Sciences, Belgrade, Serbia,* ⁵*Serbian Academy of Sciences and Arts, Belgrade, Serbia*

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¹University of Banja Luka, Faculty of Science, Banja Luka, Bosnia and Herzegovina, ²IChTM, University of Belgrade, Department of Catalysis and Chemical Engineering, Belgrade, Serbia, ³IChTM, University of Belgrade, Department of Chemistry, Belgrade, Serbia
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¹Faculty of Agriculture, Zemun, Serbia, ²Faculty of Chemistry, Belgrade, Serbia, ³Institute of Geology and Geochemistry of Petroleum and Coal, RWTH Aachen University, Aachen, Germany

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¹Vinča Institute of Nuclear Sciences, Belgrade, Serbia, ²Faculty of Mechanical Engineering, Belgrade, Serbia, ³Institute for testing materials-IMS, Belgrade, Serbia, ⁴Faculty of Technology and Metallurgy, Belgrade, Serbia
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¹UNO-LUX NS d. o. o., Belgrade, Serbia, ²Institute for Multidisciplinary Research, Belgrade, Serbia, ³The "Vinča" Institute of Nuclear Sciences, Belgrade, Serbia, ⁴Faculty of Mechanical Engineering Kraljevo, Department of Applied Mechanics, Mathematics and Physics, University of Kragujevac, Kraljevo, Serbia, ⁵Faculty of Electrical Engineering, University of Belgrade, Belgrade, Serbia

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¹*CENIMAT/I3N, Faculdade de Ciências e Tecnologia (FCT), UNL, Monte de Caparica, Portugal,* ²*"Politehnica" University of Timisoara, Timisoara, Romania*
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D. Hauserova¹, Z. Novy¹, J. Dlouhy¹, B. Masek²

¹COMTES FHT, Dobruany, Czech Republic, ²FORTECH, Pilsen, Czech Republic

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¹Karlsruhe Institute of Technology, Karlsruhe, Germany, ²Slovak Academy of Sciences, Košice, Slovakia, ³Volkswagen AG, Wolfsburg, Germany, ⁴Leibniz University Hannover, Hannover, Germany, ⁵Braunschweig University of Technology, Braunschweig, Germany
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²*Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,* ³*National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA, USA*
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¹*Faculty of Physical Chemistry, Belgrade, Serbia,* ²*Faculty of Chemistry, Belgrade, Serbia*

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¹Faculty of Pharmacy, Belgrade, Serbia, ²Faculty of Physical Chemistry, Belgrade, Serbia
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¹Alumina factory „Birac“, Zvornik, Republic of Srpska, Bosnia and Hercegovina,
²Faculty of Technology, Zvornik, Republic of Srpska, Bosnia and Hercegovina,
³Department of Materials Engineering, Faculty of Technology, Novi Sad, Serbia
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Technical University of Berlin, Department of Chemistry, Berlin, Germany
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I.M.Frantsevych Institute for Problems in Material Science of NAS of Ukraine, Kyiv, Ukraine

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Lj.M. Vračar⁵, N.V. Krstajić⁵

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¹University of Banja Luka, Medical Faculty, Republic of Srpska – BiH, ²University of Banja Luka, Faculty of Technology, Republic of Srpska – BiH, ³University of East Sarajevo, Faculty of Technology, Republic of Srpska – BiH, ⁴University of Novi Sad, Faculty of Sciences, Department of Physics, Vojvodina – Serbia, [†]Academy of Sciences and Arts of the Republic of Srpska – BiH

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Technical University of Kosice, Civil Engineering Faculty, Institute of Building and Environmental Engineering, Kosice, Slovak Republic
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Z. Ajduković¹, J. Milićević¹, M.B. Petrović¹, N. Djordjević², N. Ignjatović³, V. Savić⁴, D. Uskoković³
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M.B. Plavšić, I. Pajić-Lijaković, B. Bugarski
Faculty of Technology and Metallurgy, Belgrade University, Belgrade, Serbia
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Abstracts

Oral Presentation

PL.S.I.1

A LOOK AT NANOTECHNOLOGY: PAST, PRESENT, FUTURE

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Great strides have been made worldwide over the past two decades in our ability to create nanostructured materials and devices with novel properties and functionalities. The novel properties of these nanostructures, which provide the basis for nanotechnology, are derived from the confined sizes and very large surface-to-volume ratios of their nanoscale constituents. The former give rise to unique size-dependent properties in the nanoscale (1-100 nm) regime, while the latter give rise to the ability of nanoscale additions to conventional material matrices to dramatically change the host material's properties. Examples are nanomaterials that possess enhanced mechanical, electrical, optical, and bioactive properties, as well as multifunctional combinations thereof. A perspective of this important and still rapidly growing research area will be presented using specific examples of nanomaterials constituted of nanoparticles, nanotubes, and hybrid structures containing these and biomolecules. Opportunities and challenges facing the worldwide research community in nanomaterials and nanotechnology will be considered.

PL.S.I.2

THE IMPACT OF TRIPLE LINES ON MATERIALS SCIENCE AND ENGINEERING

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We assess the impact of triple lines in materials preparation and use by considering several examples of materials behavior in which they have identifiable effects. Like grain boundaries, their impact can far exceed their volume-fraction in a polycrystal, but generally increases with decreasing grain size, or increasing volume fraction. It is shown that the effects of triple lines can be divided into three distinct categories: (1) Cases in which the behavior of the triple line depends only upon the properties of the interfaces which it joins, and all properties of the triple line can be derived from the properties of the interfaces. (This is the conventional viewpoint for most purposes.) (2) Cases in which the termination of an interface, either internally or at a surface, changes the nature or behavior of the interface, so the introduction of a triple line changes the nature of at least one of the interfaces that it joins. (3) Cases in which the triple line has distinct properties and behaviors of its own, associated with its specific structure and interatomic bonding. We consider the impact of triple junctions on deformation, diffusion, segregation, and grain boundary migration, along with the question of triple line energy. In each case we illustrate how the behaviors and effects fall into one of the three categories above, and how this determines the appropriate level of structure to be addressed in identifying structure-property relationships.

PL.S.I.3

BIO-INSPIRED STRUCTURAL MATERIALS

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The structure of materials defines their mechanical behavior. However, in most materials, mechanical properties are controlled by structure at widely differing length scales. Nowhere is this more apparent than with biological materials, which are sophisticated composites whose unique combination of properties derives from architectural design that spans nano- to macro-scale dimensions. Few structural materials have such a hierarchy of structure, yet the message from biology is clear: superior properties can be achieved through combinations of mechanisms acting at multiple length-scales. Nature has used this approach for billions of years, yet despite intense scientific interest, the biomimetic approach has yielded few technological advances in the design of new synthetic structural materials primarily because they are difficult to fabricate and there is still lack of understanding of the salient toughening mechanisms involved. Here we describe the origin of toughening in several important biological materials, including bone, tooth dentin and mollusk shells. Based on this understanding, we attempt to emulate Nature's toughening mechanisms using a freeze-casting fabrication process to make materials through the combination of two ordinary compounds, specifically alumina and PMMA, into ice-templated structures whose toughness can be over 300 times (in energy terms) that of their constituents. The final products are bulk, lightweight, hierarchical hybrid ceramic-based materials whose mechanical properties represent the highest toughness ceramics ever produced; indeed, their specific properties are comparable to metallic aluminum alloys. These materials are unlike regular composites in that both phases are not load-bearing; the ceramic phase provides for strength but the polymer phase acts like a lubricant to relieve high stresses, much like plasticity in metals.

PL.S.I.4

**RECENT ELECTRON MICROSCOPE STUDIES OF GOLD-BASED
NANOPARTICLES FOR MEDICAL APPLICATIONS**

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We have extended our previous work on silver-based surface enhanced Raman spectroscopy nanoparticles to silica-coated gold nanoparticles. Various scanning electron microscopy techniques are used to show how the particles attach to cells. The fine structure of the particles is more clearly revealed by transmission electron microscopy. Moreover, scanning transmission electron microscopy is very useful in examining large volumes of rat liver to establish whether these nanoparticles have reached this organ after venal injection. The importance of this work for possible medical applications will be discussed.

PL.S.I.5

**CONVERGING THEORY AND EXPERIMENT: NUCLEATION OF $L1_2$ COMPLEX
NANOSTRUCTURES**

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Al-Li alloys are of great interest for aerospace and cryogenic applications due to their low density and high strength-to-weight ratio. The mechanical properties of these alloys are based on a fine dispersion of coherent Al_3Li metastable precipitates formed by congruent ordering and spinodal decomposition. Other elements, such as Sc and Zr, are added to Al-Li alloys to further improve their properties. These alloys were found to contain a fine distribution of remarkably monodisperse core/shell precipitates consisting of an Al_3ScLi core surrounded by a shell of pure Al_3Li , with Zr segregating at the core/shell interface. Monodisperse Al_3ScLi core/shell ordered precipitates with a Sc and Li-rich core surrounded by a Li-rich shell can be created via a three-stage heat treatment. The atomic structure of these precipitates has been studied by a range of advanced microscopy, spectroscopy and synchrotron radiation techniques combined with first-principles calculations of interaction between Sc and Li confined in the ordered structure. Conventional high-resolution phase contrast imaging reveals the fully ordered $L1_2$ structure of the shell. Atom-probe tomography reveals that Sc is present in the core while Li is present in both, the core and the shell. Aberration corrected transmission electron microscopy was employed to image Li using exit wave reconstruction. The phase of the exit wave distinguished clearly Al columns from Li columns in the Li rich $L1_2$ shell. A detailed analysis of these precipitates has provided important insights into their atomic structure and composition. This work is supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

O.S.A.1

INFLUENCE OF IRRADIATION DEFECTS ON THE STRENGTH OF COPPER AT A NANOMETER SCALE

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We investigate the influence of irradiation defects on the size dependent mechanical properties of single crystal copper oriented for multiple slip deformation. Single crystal wedges were cut from bulk single crystals, grinded, electro-chemically etched, and partly irradiated to 1 dpa using a high energy proton beam. A focused ion beam microscope was utilized to machine compression samples with diameters ranging from 100 nm up to 1 μ m into these wedges. Subsequently, the samples were tested in situ in a Jeol 3010 TEM using a nanoindentation holder outfitted with a flat diamond tip. The results show a transition in deformation mode for the irradiated material. For larger sample diameters the strength is found to be size independent, governed by defect-dislocation interaction. For smaller samples the yield strength was found to be size dependent, limited by the strength of available dislocation sources.

O.S.A.2

STRUCTURE PREDICTION FOR PbS AND ZnO AT DIFFERENT PRESSURES AND VISUALIZATION OF THE ENERGY LANDSCAPES

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An important issue in modern solid state chemistry is the development of a general methodology to predict the possible (meta)-stable modifications of a solid. This requires the global exploration of the energy landscape of the chemical system, since each stable phase corresponds to a locally ergodic region of the landscape. The global search in the lead sulfide system has been performed with simulated annealing (SA) on the ab initio level, while zinc oxide was studied with an empirical potential using SA, both at standard and elevated pressure (up to 100 GPa). The local optimization of the modifications found in the PbS system was performed using various density functionals. Next, the E(V) and H(p) curves were computed for these modifications and their electronic structure was analyzed. The structures found for ZnO were locally optimized on ab initio level (DFT and Hartree-Fock). In both systems the structures found were in good agreement with the experiment. Furthermore, we employed the threshold algorithm (TA) to explore the barrier structure of the landscape of ZnO as function of the number of formula units in the simulation cell. Based on the barrier and minima information, both tree models and 2D- models of the energy landscape were constructed.

O.S.A.3

HIGH-TEMPERATURE OPTICAL IN-SITU STUDIES OF REDOX PROCESSES IN COMPLEX OXIDES

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Oxidation and reduction of oxides represent an important class of reactive solid state processes associated with the attainment of crystal stoichiometry and many other important materials properties. In the present study, optical spectroscopy is used to detect such processes under in-situ conditions at elevated temperatures. Due to defect-induced optical absorption, experiments performed at different oxygen activities provide information on the oxygen activity dependence of defect concentrations. The kinetics of redox processes is studied by means of oxygen activity-jump relaxation experiments. In the present contribution, results are reported for redox processes in cobalt-containing olivine single crystals (Co_2SiO_4) at temperatures ranging between 750 and 1010°C and in cerium-containing yttria stabilized zirconia (Ce:YSZ).

O.S.A.4

MECHANOCHEMICAL PREPARATION OF ORGANIC-INORGANIC HYBRID MATERIALS OF DRUGS WITH INORGANIC OXIDES

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The composites of piroxicam and meloxicam with alumina and ferric oxide were prepared by mechanochemical method. Electron microscopy studies showed the formation of a nano-sized layer of the drugs at the surface of the oxide. The changes in the IR spectra suggested the interaction of the components during co-grinding. The data of X-ray photoelectronic spectroscopy confirmed the interaction of the functional groups of the drug with the surface of alumina. The formation of new bonds at the contact of particles in the composite leads to stabilization of drugs in a metastable state inhibiting their crystallization and transition into initial crystalline form. The nanocomposites obtained revealed the controlled drug release. Incorporated with magnetic nanoparticles they can be used for targeted release also. The work was supported by the grants of CRDF (RUX0-008-NO-06) and RFBR (09-03-92658).

O.S.A.5

**REGULARITIES OF FORMATION, STRUCTURE AND CHEMICAL PROPERTIES
OF NANOSIZED MoO₃ AND Me/MoO₃ (Me=Al, Mg, Si) NANOCOMPOSITES,
PREPARED BY MECHANOCHEMICAL METHOD**

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Mechanical activation of energetic composites metal/solid oxidizer Me/MoO₃ (Me=Al, Mg, Si), leads to formation of nanocomposites, which demonstrate high burning or detonation velocities. The paper devotes to the regularities of MoO₃ nanoparticles and MoO₃ based nanocomposites formation under mechanical activation and their physical and chemical properties. Mechanical activation was done in the vibrating mill in inert atmosphere with/without liquid additives (hexane). The structure of activated samples were investigated by the methods of X-Ray diffraction (XRD), Scanning Electron Microscopy (SEM), Atom Force microscopy (AFM), laser diffraction particle size analysis, DTG and adsorption. There are two main stages of mechanical activation of MoO₃. The formation of MoO₃ nano dimension particles with average size close to 60 nm and specific surface area 25 m²/g is the result of the first stage. Formed nanoparticles had layer structure with characteristic size 25-30 nm. The second stage is accumulation of defect structure (microdistortions) prior in the direction (100) and partial mechanochemical decomposition (reduction) of oxide. The second stage was conveyed by aggregation of particles and decrease of specific surface area. Under the mechanical activation in presence of hexane only the splitting of particles took place, but the rate of destruction in this case significantly low than under mechanical treatment without hexane. It was developed the two stages method of mechanical activation of Me/MoO₃ (1-st stage is mechanochemical preparation of nano-MoO₃, 2-d stage is activation Me+nano MoO₃). The formation kinetics, structure and burning properties of nananocomposites Mg/MoO₃, AlMoO₃ and Si/MoO₃ were compared. This work was partly supported by RFBR (projects No 10-03-00942a, No 09-03-00409a and No 10-03-09909a), and Program No 18 of Fundamental Investigation of Presidium RAS.

O.S.A.6

**BULK AMORPHOUS CU- AND NI- BASED ALLOYS PROCESSED
BY MECHANICAL ALLOYING AND POWDER COMPACTION**

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Bulk metallic glasses (BMG) are new group of materials widely studied mainly due to their good mechanical properties and corrosion resistance. Usually BMG are fabricated from the liquid state by mould casting. However, there is an alternative method of producing of bulk amorphous alloys – by compaction of amorphous alloyed powders. Such powders can be obtained by atomization or by mechanical alloying technique. The aim of this study was to fabricate by mechanical alloying selected CuTiNiZr and NiTiZr alloys with other additions (Sn, Ag). Next, structural studies were performed in order to determine the influence of chemical composition on amorphization and thermal stability of the alloys. The powders were compacted and selected mechanical properties of bulk alloys were determined.

O.S.A.7

SYNTHESIS AND CHARACTERIZATION OF NiMn_xFe_{2-x}O₄ FERRITES

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Ferrites of nominal composition NiMn_xFe_{1-x}O₄, with $x = 0 \div 1.0$ have been synthesized by self-propagating high-temperature synthesis. The products of synthesis had small variations in phase compositions that had been eliminated after thermal treatment at 1270 K during 50 min. With manganese content (x) increase lattice constant of the ferrites gradually increases from 0.833896 nm (x=0) up to 0.836369 nm (x=1). The obtained powder product contains two types of ferrite particles that are varied in size and form. At the same time magnetic properties depend significantly on microstructure and chemical composition of synthesized ferrites. For coercive force it has been observed the increase of H_c value from 1.75 (x= 0.2) to 2.85 (x= 1) due to products microstructure.

O.S.A.8

SINTERING OF DEFECT-FREE BTS2.5/BTS5/BTS7/BTS10 FUNCTIONALLY GRADED MATERIALS

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As continue of our previous studies, four component barium titanate-stannate ($\text{BaTi}_{1-x}\text{Sn}_x\text{O}_3$, BTS) functionally graded materials (FGMs) were designed and examined. BTS powders with different tin content ($\text{BaTi}_{0.975}\text{Sn}_{0.025}\text{O}_3$, $\text{BaTi}_{0.95}\text{Sn}_{0.05}\text{O}_3$, $\text{BaTi}_{0.93}\text{Sn}_{0.07}\text{O}_3$ and $\text{BaTi}_{0.9}\text{Sn}_{0.1}\text{O}_3$, denoted as BTS2.5, BTS5, BTS7 and BTS10, respectively) were used. Four layered samples, produced by powder-stacking method and uniaxially-pressing process, were transformed in BTS2.5/BTS5/BTS7/BTS10 FGMs by sintering at 1420 °C during two hours. It is known that during sintering of FGMs, different BTS powders can show different shrinkage extents, as well as different final density, which can lead to excessive shape distortion, warping, delamination, crack development and microstructural damage in the FGMs. Thus, to achieve high-quality FGMs, without above listed disadvantages, we used the master sintering curve (MSC) approach. In this study, the MSCs were constructed for FGMs using shrinkage data obtained by a heating microscope during non-isothermal sintering up to 1420 °C with heating rates of, 2, 5, 10 and 30 °/min. For wished density value (ordinate of the created MSCs graph) appropriate θ value was found (reading from the MSCs abscissa), yielding heating rate that should be applied during sintering to obtained FGMs with desired density. Finally, estimated heating rate was applied, and defect-free BTS2.5/BTS5/BTS7/BTS10 FGM with desired microstructure was prepared. The microstructure and chemical (Ti/Sn) gradient in the prepared FGMs were examined by FESEM-EDS methods.

O.S.A.9

**MICROWAVE ASSISTED SOLVENT FREE REACTIONS OF SOME
INTERCALATIVE COMPOUNDS AND PHTHALOCYANINE DERIVATIVES**

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It is well known that many reactions occur in a solid state efficiently. It means that the reacting molecules are able to move freely in the solid state. It is extremely difficult to carry out solid-state chemical reactions under microwave activation. The reaction course will be effective providing greater surface contact of the reacting components. The microwave-heating rate has a strong functional relationship to the dielectric properties (particularly dipole mobility) and electric field strength. From this perspective, the efficiency of microwave radiation absorption should be minimal for solid organic and inorganic compounds. We have investigated features of microwave absorption for certain intercalative compounds with organic reagents as well as for some solid organic compounds. Another direction of our study was microwave-assisted synthesis of some phthalocyanine derivatives. The synthesis were carried out using microwave system 'Explorer-48', equipped with video camera. This accessory provided video recording of changes of reactants due to microwave irradiation. It was found the effectiveness of microwave heating for fluorinated graphite intercalation compounds depends on the dielectric properties of the organic reagent embedded. After the decomposition of these compounds and the formation of nanostructured carbon, the appearance of high-frequency corona discharge on carbon fibers was recorded using video camera. The formation of high-frequency discharge explains features of temperature fluctuations in the sample. On the other hand, this is an indication of high-density microwave energy in the cylindrical resonator of our microwave system. However, heating of organic and inorganic compounds in the solid phase is extremely slow and requires high power microwave exposure. The sharp rise in temperature and microwave power reset occurs only after melting at least one of the reactant. This fact was confirmed by video recording of the reaction in the microwave cell. The microwave synthesis of Cu, Zn phthalocyanine derivatives occurred under high speed only after the formation of the melting phase. The yield was improved in 3-4 times, and the reaction time was reduced more than two orders of magnitude. Consequently, the microwave irradiation method provided higher product yields in a very short period of time. These results suggest the method was more useful in compare with the conventional method due to shorter reaction time and energy savings. However, reactions in the solid phase are practically impossible for microwave systems, without intensive mixing of solid reagents, so the process is effective only in the molten state.

O.S.A.10

**PREPARATION OF LiFePO₄/C COMPOSITES BY CO-PRECIPITATION
IN THE PRESENCE OF STEARIC ACID**

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The olivine type compositions LiMPO₄ (M = Fe, Mn, Co) are among the most attractive materials for the positive electrode of lithium-ion battery. The benefits of using LiFePO₄ are excellent cycle life, high structural stability, low cost and environmental friendliness. Its main limitation is low total electrical conductivity, which can be overcome by carbon coating and/or the achievement of a small and homogeneous particle size distribution. Here is presented a simple and inexpensive route for obtaining LiFePO₄/C composites by aqueous co-precipitation of an Fe(II) precursor material in the presence of stearic acid and subsequent heat treatment at different temperatures. Stearic acid serves as both chelating agent and carbonaceous material. During pyrolytic degradation stearic acid decomposes to carbon while creating reductive atmosphere. The crystal structures of the powders were revealed by X-ray powder diffraction. It was shown that phase purity of the synthesized powders is very dependent on calcination temperature, as well as their electrochemical properties.

O.S.A.11

**PREPARATION AND SURFACE PROPERTIES
OF CeO₂-Nb₂O₅ MIXED-OXIDE CATALYSTS**

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The present work is focused on the synthesis and characterization of ceria-niobia mixed oxides. Mixed oxides with a wide range of niobia content were prepared by coprecipitation method with the aim to obtain given acid-base characteristics and subsequently to investigate the catalytic properties of the obtained materials. The synthesized solids have been characterized in terms of their structural, textural, and surface properties, including the acid-base and red-ox features, by a variety of techniques (BET, XRD, Raman spectroscopy, TG, and TPR-TPO). The acid-base properties were estimated by adsorption microcalorimetry measurements of ammonia and sulfur dioxide. All obtained mixed oxides showed specific amphoteric character influenced by relative amounts of the two component oxides. The obtained materials exhibited satisfactory homogeneity; the highest surface area was achieved for sample containing 73 wt % of CeO₂. Only the fluorite structure of CeO₂ was observed by XRD for all prepared mixed oxides. The crystallinity of samples decreased with increasing amount of Nb₂O₅. TPR-TPO results were strongly dependent on the bonding nature between the two oxides. In conclusion it was possible to tune the number of surface active sites by varying the ratio of ceria to niobia.

O.S.A.12

PHOTOCATALYTIC ACTIVITY OF PHOSPHATED TiO₂ NANOPOWDERS

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The photocatalytic activity of TiO₂ synthesized by combination of sol-gel and solvothermal synthesis was improved by phosphorous (P) incorporation. Samples were characterized by means of X-ray powder diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). The specific surface area was measured with the Brunauer-Emmet-Teller (BET) method and the photocatalytic activity of the samples was evaluated as velocity of the acetone formation from isopropanol. So prepared TiO₂ crystallized as nano-crystalline anatase powder with high specific surface area (up to 335 m²/g). Phosphorous incorporation inhibits grain growth and stabilizes anatase phase up to higher temperatures. It was observed that photocatalytic efficiency of phosphorous containing TiO₂ is higher in comparison with anatase without phosphorous.

O.S.A.13

**HIGH VELOCITY SUSPENSION FLAME SPRAYING (HVSFS);
PROCESS DEVELOPMENT AND INDUSTRIAL APPLICATIONS**

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Thermal spraying of suspensions containing oxide ceramic particles of micron, submicron or nano scale offers new possibilities in functional coating development and opens up new application fields. Regarding their mechanical and physical properties, suspension sprayed coatings differ significantly from conventionally sprayed, mainly due to their refined microstructure. Dense coatings with a refined microstructure and a layer thickness typically ranging from 10 – 200 μm can be achieved. Thus, HVSFS can close the gap between conventional spray coatings (APS, HVOF) and thin film technology (CVD, PVD). The presentation will introduce the process, discuss suspension preparation and their related properties and will give some potential application examples.

O.S.A.14

SUPERELASTIC BEHAVIOUR OF LASER WELDED JOINTS IN NiTi

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NiTi is known for its shape memory effect and superelasticity. Its reduced workability by conventional machining processes and increasing fields of industrial application demands suitable joining techniques in order to obtain complex components. It is well known that fusion welding reduces the shape memory effect due to structural modifications, but there is no systematic study on its influence on the superelasticity.

This paper presents results of CW Nd/YAG laser similar welding of butt joints regarding superelastic behaviour. Though the results indicate that laser welding of NiTi specimens reduce the mechanical strength under tensile loads, good hysteretic cycling behaviour can be achieved at stress levels corresponding to the yield plateau of the base material.

O.S.A.15

La_{1-x}Ca_xFeO₃ HOMOGENEOUS AND MICROHETEROGENEOUS PEROVSKITE-LIKE OXIDES: SYNTHESIS, MICROSTRUCTURE, STABILITY AND CATALYTIC ACTIVITY

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This work presents results of research aimed at elucidating general trends in formation of the phase composition and microstructure of Ca doped lanthanum ferrites - La_{1-x}Ca_xFeO_{3±δ} prepared via the mechanochemical and Pechini routes. Combination of diffraction (X-ray diffraction including high temperature investigation, transmission electron microscopy) and spectroscopic methods (Infra-red spectroscopy, Mössbauer spectroscopy) with temperature-programmed techniques (thermal analysis, reduction by H₂) allowed to clarify the effect of the preparation route and content of a dopant on the charge state and coordination of Fe cations determining in turn mobility and reactivity of the surface and lattice oxygen and catalytic activity. For mechanochemical route of La_{1-x}Ca_xFeO₃ ferrites synthesis, microheterogeneous/nanocomposites solid solutions and for Pechini route homogeneous solid solutions were obtained and their stability at high temperatures in the air and in the vacuum were determined as well as surface and bulk oxygen reactivity. This allowed obtaining complex perovskite-like ferrites with controlled properties required for application in a high-temperature oxidation catalytic process (methane combustion, ammonia oxidation et al).

Key words: mechanochemical synthesis, Pechini synthesis, perovskites, microstructure, properties.

O.S.B.1

**RETENTION OF COLLOIDAL CdS NANOCRYSTALS
BY SILICON MOLECULAR FILTER DURING ELECTROPHORESIS**

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When investigating electrophoresis of CdS nanoparticles through a silicon molecular filter, retention effect has been observed. These nanoparticles were CdS nanocrystals with a diameter of 3.12 nm which were encapsulated in thioglycolic acid (TGA) shell of a thickness around 0.5 nm. The molecular filter consisted of a porous amorphous silicon plasmochemically deposited on a microchannel membrane as a continuous layer. After each consecutive electrophoresis operation absorption lines of TGA in obtained IR-spectra of the filter indicated of nanoparticles concentration on/in the filter. Structural analysis results became direct evidence of the retention effect of CdS nanoparticles by the molecular filter during electrophoresis. They showed a presence of nanocrystals on the filter surface.

O.S.B.2

**COMPOSITION, ATOMIC STRUCTURE AND ELECTRONIC PROPERTIES
OF FLUORINE PASSIVATED InAs (111)A/ANODIC OXIDE INTERFACE**

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The atomic structure of semiconductor A_3B_5 /oxide interface is a crucial to understand the interfacial electrical properties. The aim of this work is to elucidate the mechanism of decrease density of interfacial states ($<5 \cdot 10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$) in InAs (111)A/oxyfluoride anodic films (OAF). The comparative study of phase composition of OAF (formed in electrolyte with different pH and F^- concentration) by XPS shown that fluorination leads to formation InAs/InF₃ interface and As⁵⁺ oxidation forms in OAF as compared to InAs/(In₂O₃+A₂O₃) interface without fluorine. This result was confirmed by estimating of oxygen and fluorine influence on the changing of electronic states of In-terminated InAs surface by the first-principles calculation: the In-top position of fluorine is preferable. Adsorption of fluorine in this position leads to removal electronic states in the energy gap.

O.S.B.3

**NEW COMPOSITE CERAMIC MATERIALS FOR PVD TARGETS BASED ON
Ti-Al-Si₃N₄-C SYSTEM PRODUCED BY COMBUSTION SYNTHESIS**

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This paper is devoted to production of new composite ceramic materials based on Ti-Al-Si₃N₄-C system by self-propagating high-temperature synthesis (SHS). Green mixtures were prepared from elemental powders of Ti, Al, C (carbon black) and Si₃N₄ using a ball mill. Compositions of the green mixtures can be described by the following equation: $X[\text{Ti}+3\text{Al}]+(100-X)[0,448(2\text{Ti}+\text{C})+0,552(5\text{Ti}+\text{Si}_3\text{N}_4+4\text{Al})]$, where X is a mixture parameter from 10 % to 50 %. Macrokinetics of the combustion process has been investigated in dependence of mixture composition and initial conditions of SHS-process. It was determined that increase in mixture parameter (X) leads to decrease of the combustion temperature and rate, because of changing of leading chemical reaction during combustion process. But also the increase in initial temperature of SHS- process from 25 °C up to 350 °C promotes to increasing of the combustion temperature (on 200 °C in average) and combustion rate (in two times). Compact samples of the composite ceramic materials were produced by force SHS- pressing technique. The phase composition and structure of the synthesis products has been investigated using x-ray diffraction (XRD), optical and scanning electron microscopy (SEM). It was obtained by XRD that the main phase in the final SHS- products composition with mixture parameter X = 10, 20 and 28,1 % is Ti(C,N), and its also includes two binder phases TiAl₃ and Ti₅Si₃. The main phase in phase composition of ceramic materials with mixture parameter X = 40 and 50 % is intermetallide TiAl₃. It was shown that the increase in mixture parameter leads to decrease of the Ti(C,N) and Ti₅Si₃ content and promotes to increase of TiAl₃ amount in the synthesis products. The new phase Ti₃SiC₂ with laminated structure appeared in materials with X = 28,1 and 40 % in amount of 10 and 39 % respectively. Complex investigations of physical (density, residual porosity, sonic rate) and mechanical (Young modulus, bending strength, Vickers hardness) properties of new composite ceramic materials in Ti-Al-Si₃N₄-C system were carried out at present study. The opposite dependence between density, Vickers hardness and mixture parameter was determined. Investigated ceramic materials had a density values of 3,2 ~ 4,2 g/cm³, residual porosity 0,5 ~ 4,0 % and displayed a Vickers hardness values from 7,4 to 10,3 GPa, bending strength 182 ~ 218 MPa and Young modulus 385 ~ 521 GPa. Fabricated ceramic materials based on titanium carbonitride, silicide and aluminide are very attractive for practical application as a targets material for deposition of a nanostructured coatings possessed of high values of wear-, corrosion- and heat resistance and reduced friction coefficient on different substrates by magnetron sputtering technique.

O.S.B.4

THE STRUCTURAL ATOMIC MODELS OF W/Si INTERFACES AND PROCESSES OF SELF-ORGANIZATION OF INTERFACE REACTION ZONE IN CVD GROWTH OF TUNGSTEN THIN-FILMS ON SILICON SUBSTRATE

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Interface modeling, thermodynamic considerations and study of the self-organization phenomenon of reaction zone are applied to optimization of chemical vapour deposition (CVD) of tungsten thin-films on silicon substrate. Tungsten films are perspective materials of multilayered contact metallization of integrated circuits. The main difficulties in fabricating of the W thin-film microstructures are sufficiently low adhesion to silicon and spalling of metal layers. The films were obtained with the use of various techniques: CVD technique by the hydrogen reduction of tungsten hexafluoride, CVD with the plasmochemical stimulation of hydrogen and magnetron sputtering. It was discovered that only in the CVD-process the W_5Si_3 self-limited nanometric sublayer tungsten silicide is formed at the interface W/Si. The low pressure, low temperature CVD of tungsten films is non equilibrium process with many variable growth parameters. The nucleation of new phase at the interface is determined by the composition of intermediate interfacial layer (reaction zone), which possibly regulate by reagent flows in CVD and by the energy necessary to form the compound. On the basis of the thermodynamic analysis of effective heat of compound formation as function of concentration of reacting components in reaction zone and kinetic model of tungsten film formation on the Si substrate from gas phase WF_6/H_2 in the CVD-process, the conditions for preferential formation of the W_5Si_3 silicide in comparison with disilicide WSi_2 were determined. Alongside with thermodynamic and kinetic factors there are very important structure and energy of interfaces formed during CVD. According calculations of elastic strains and interface structural models it was shown, that sublayer W_5Si_3 has structural conformity (lattice matching) both to W, and to Si and acts as adhesive promoter. Up to the definite thickness (~ 20 nm) more dense structure of W_5Si_3 (compared with WSi_2) serves as an effective diffusion barrier for formation of other silicides with higher silicon content that leads to sharp decrease in conductivity. The energy nanosystem stabilization and formation of low-energy coherent interfaces are driving forces of the CVD of tungsten thin-films. The matching of the CVD technique with the processes of internal structural self-organization of the system allow us to obtain high-conducting, structurally stable thin film nanostructures of W on Si substrates.

O.S.B.5

SHS METALLURGY OF CAST ALLOYS UNDER HIGH GRAVITY

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The work is aimed at developing a new technology for obtaining multicomponent materials (metallic alloys) by SHS metallurgy. In overall view the chemical scheme for obtaining of cast polymetallic alloys by means SHS metallurgy can be represented as:

$(Ox_1 + Ox_2 + Ox_3 + \dots Ox_n) + R \rightarrow [\text{multicomponent alloy}] + R_kO_l + Q$, where Ox_i – oxides of Ni, Co, Mn and so on, R – metal reducer (Al), [polymetallic alloy] – (Ni, Co, Mn)Al_x, Q – thermal effect of the process. Owing to exothermic reactions of metal oxides reducing and SHS reactions for intermetallic formation provides melt final products consisting of polymetallic alloys (bottom layer) and metal reduce oxide (upper layer). A short time synthesis and protection of the metal melt from oxidation by Al₂O₃ melt permit to obtain the alloys in air atmosphere. The main advantages of the technology include low energy costs, higher productivity (due to the small-time synthesis, 1-60 sec), the use of cheaper raw materials (metal oxides) and the use of cheaper equipment. Realization of high temperatures without using any additional power sources is the basic difference of the SHS from the conventional vacuum electrometallurgy. The composition/structure of SHS-produced cast multicomponent Co, Ni and Ti based alloys in centrifuges was found to depend on the extent of centrifugal overload *a/g*. created in the centrifugal SHS installations. Therefore burning of initial compositions performed under high gravity (*centrifugal force*). The obtained cast alloys have high level of homogenization and fine-grained structure. The pilot series of cast SHS alloys were produced for various application including heat-resistant alloys, masteralloys, intermetallic alloys, etc.

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O.S.B.6

**Co-B CATALYSTS FOR HYDROLYSIS OF BORON-BASED COMPLEX HYDRIDES
TO GENERATE PURE HYDROGEN FOR PEM FUEL CELL**

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Today, hydrogen storage is one of the most important issues that hinder the development of a hydrogen economy. Many studies searching for effective storage materials are in progress but none has reached the technical criteria that could make them viable from the technological and commercial points of view. According to many researchers, hydrogen generators based on hydrolysis of hydrides are offered as promising portable devices that were employed with proton-exchange fuel cells. Among the hydrides, sodium borohydride (10.5 wt% H) and ammonia-borane (19.4 wt% H) are desirable due to the high hydrogen content and the high stability. Today, most of the published papers about the NaBH₄ and NH₃BH₃ hydrolysis deal with improvement of catalytic materials. The most efficient metals (supported or not) are the noble metals. A non-noble metal, cobalt, has showed promising catalytic performances and many studies have then focused on improving its reactivity. Also, the problem of macrostructured catalysts creation (in the form of granules and blocks) needed for the flow operation of portable hydrogen generator is still unsolved. In this work, hydrogen generation from NaBH₄ and NH₃BH₃ have been studied in the presence of different nanoscale catalysts (supported or not) containing Pt, Ru, Rh, Co, Ni. Different methods (magnetic susceptibility measurement, XRD, FTIR, DRS, TEM, et. al.) were used for catalysts study. By varying the conditions of the catalyst preparation and the nature of the active component and support it was possible to control the properties of the hydrogen-generating systems and the rate of the process. Low cost of cobalt catalysts is very attractive in developing on-demand hydrogen generation system for practical application. Different cobalt salts, cobalt hydroxide and Co₃O₄ were investigated as catalytic materials for the hydrolysis of boron-based complex hydrides. During the investigation, it was found that cobalt-based catalysts were reduced in the reaction media of boron-containing hydrides to form the active ferromagnetic phase of Co_xB. Cobalt-based catalyst ferromagnetism makes it convenient for easy catalyst separation from reaction products and for development of new types of catalytic reactors for portable applications. The data of the study of dependence of the catalytic samples magnetic susceptibility values on temperature lead to conclusion that active catalytic phase is Co₂B. Moreover, catalytic samples prepared from Co₃O₄ are characterized with high magnetic susceptibility value and high level of catalytic activity. It was shown that structured catalysts can be used in portable H₂ generator. Methods of macrostructured catalysts preparation have been developed. Using cobalt borides supported on Ni-foam allows us to achieve next advantages: strength support, low hydrodynamic and aerodynamic resistance, easy separation of spent solutions.

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O.S.B.7

DEVELOPMENT OF NEW TOOL STEELS FOR FORGING DIES

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Forging dies used for close dies forging of small and middle-sized steel parts are required to possess an optimum combination of strength, toughness, resistance to tempering and other properties. Typical alloying elements include chromium, vanadium, molybdenum, or tungsten. This alloying strategy can be found e.g. in the steels 1.2343, 1.2344 and others.

The present paper describes new alloying concepts of steels for forging dies based on the 1.2343 steel. By increasing the carbon content, and in some cases increasing the tungsten level and adding niobium, using a sufficient metallurgical procedure and subsequent special process for ingot forging, the hardness, toughness and wear resistance of the steel have been enhanced significantly. The lifetime of dies made from the improved steels is about 50-100% longer than that of dies made from conventional 1.2343 steel.

O.S.B.8

INFLUENCE OF CASTING PARAMETERS ON GLASS FORMING ABILITY AND MECHANICAL PROPERTIES OF $Zr_{48}Cu_{36}Ag_8Al_8$ BULK METALLIC GLASS

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The properties of bulk metallic glasses (BMG) are sensitive for parameters related to technological process. The goal of this work was to study the influence of manufacturing conditions of $Zr_{48}Cu_{36}Ag_8Al_8$ BMG on its glass forming ability (GFA) and mechanical properties. The investigated BMG was produced by casting technique into a copper mould, manufacturing rod shape samples with different diameters. Structural characterization was performed by x-ray diffraction. The GFA of studied alloys has been investigated on the basis of some thermal stability parameters and temperature interval of supercooled liquid region. Mechanical properties were determined by Vickers microhardness measurements (50 g load) and room temperature compression tests (strain rate $10^{-4} s^{-1}$). The fracture surfaces of the samples after failure were examined by scanning electron microscopy.

O.S.B.9

**THERMAL MEMORY PROPERTIES AND DEPTH INHOMOGENITY OF
POLYOLEFINES DETERMINED BY PHOTOACOUSTIC FREQUENCY METHOD**

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In this article, we present a short review of the recent development of the theoretical model for gas-microphone photoacoustic, including thermal memory effects and the thermal depth inhomogeneity of a thin sample. Measuring of thermal relaxation time and the depth profile of thermal diffusivity of polyolefines is based on the aforementioned theoretical model and conducted on the recently developed experimental apparatus. The obtained result is very important because the one represents the first measurement of thermal memory properties in the world and their recognition is significant not only for the use of conventional polyolefines for modern applications, but also for further fundamental research.

O.S.B.10

STABLE CRACK GROWTH IN AUTOMOTIVE STEEL SHEETS

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Crack growth resistance measuring on automotive thin (1.8 mm) steel sheets. Stable crack growth was monitored with non contact videoextensometry technique on CT (Compact Tension) specimens with various notch orientation (parallel to rolling direction and perpendicular to rolling direction). Specimens were loaded under two loading rates (1.3 mm/min and 130 mm/min). CTOD (Crack Tip Opening Displacement), J-integral and crack growth Δa were specified and afterwards the R-curves were established. Determination of the plastic hinge position during loading.

O.S.B.11

CHANGES IN MICROSTRUCTURE OF AIR PLASMA SPRAYED MCrAlY COATINGS AFTER SHORT THERMAL EXPOSURE IN ARGON ATMOSPHERE

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Two NiCrAlY and CoNiCrAlY powders were used to produce the MCrAlY type of coatings by means of conventional thermal air plasma spraying on Inconel 713LC nickel-based superalloy substrate. After spraying, an initial state of both types of coatings consisted of the beta-NiAl intermediate phase, gamma-Ni solid solution and it also included a certain amount of imperfectly melted powder particles, voids and Al₂O₃ oxide particles. The coatings were annealed for two hours at wide range of the temperatures (650, 800, 1000 and 1150°C) in argon-flow atmosphere. After this short thermal exposure the changes in the microstructures were studied in detail. It was found that the temperature influences the coatings microstructure significantly. On the other hand, it has only minor effect on the coatings thickness, which is almost equal to its initial state value. At high temperatures, the oxide scale is formed by internal oxidation being the most detrimental mechanism. In the consequence, the beta-NiAl intermediate phase disappears and the gamma-Ni, alpha-Cr solid solutions and Al₂O₃ oxide starts to form within the coatings. No interaction at the coatings-substrate interfaces were observed after this short thermal exposure. The coatings' microstructure was studied by scanning electron microscope. Layer thickness and the amount of the oxide scale in coatings were measured by means of image analyses. Chemical composition was estimated by energy dispersive microanalysis measurements.

O.S.B.12

ADSORBATE – INDUCED DIGITAL ETCHING OF GaAs(001) WITH A MONOLAYER PRECISION CONTROLLED BY SURFACE RECONSTRUCTION

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Digital etching of III-V semiconductors with a monolayer precision has been realized by means of self-limiting surface reactions with adsorbates interacting selectively with atoms of group III and group V. The reversible transitions between the As-rich and Ga-rich reconstructions are experimentally observed under adsorption of cesium and iodine on the GaAs(001) surface followed by heating in vacuum at moderate temperatures T=400-450°C. The observed cesium and iodine-induced transitions between the As-rich and Ga-rich GaAs(001) surface reconstructions can be explained by adatom-induced weakening of the bonds between the uppermost layer of surface atoms with the substrate that confirmed by the results of first-principles calculations.

O.S.B.13

OVERALL MODEL OF PLASTICITY AND FAILURE OF METALS

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On the base of experimental evidence a new model of plastic flow and failure has been elaborated. The plastic flow investigations were performed for pure FCC, BCC and HCP metals and alloys in single-crystal and polycrystalline state; alkali halide crystals and some rocks were also tested. The distortion tensor components were examined by a specially developed holographic technique. It is shown that the plastic flow tends to localize on the macro-scale level. The localization phenomena are wave-like in character. The principal characteristics of these waves are determined. It is found that plastic deformation and ductile failure can be suitably approached through the concept of evolution of the said waves. It is also shown that from the macrolocalization pattern one could predict the place and instant of failure.

O.S.B.14

NANO-COATING AS A METHOD TO IMPROVE PHYSICAL AND MECHANIC CHARACTERISTICS OF MATERIALS

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The technology of high strength anti-corrosion nano-coating was developed by the Institute of High Current Electronics. The technology of nano-coating alters physical and mechanic characteristics of materials and significantly extends the operational time of objects and tools made from such materials.

This study examines both mechanic and acoustic characteristics of the aluminum alloy D1 with the various depth of nano-coating. The alloy D 1 is widely used by the industry to produce blades for the aircraft, fastening joints and parts of constructions of medium strength. The paper examines acoustic emission created during the deformation of alloy samples.

Additional distorting impulses are detected when localizing the signals of acoustic emissions in materials with nano-coating. However, these impulses do not influence the ordering of the signals of acoustic emissions until the moment of alloy's deformation. The distance between the maximums of localization remains unchanged.

The findings of the study show that the examined aluminum alloy D1 with the nano-coating has increased resistance without decrease in its plasticity characteristics. The plasticity of alloy varies with the change of the nano-coating depth and the time of the nano-coating treatment. The best results in plasticity were achieved at the nano-coating treatment for one hour. The study concludes that the mechanic features of alloys widely used in the industry can be improved by the present nano-coating technology.

PL.S.II.1

ELECTRONICALLY TUNABLE NANOSTRUCTURES

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The properties of materials are typically controlled in a static manner by their microstructure. This implies control of the grain size, defect concentration, structure and metastability. As long as the microstructure does not change during the use of the material, the properties of the material are fixed, or irreversible. In contrast, in semiconducting materials, properties can be tuned by the application of an external field due to the space charge regions which extend far from the interfaces. In metallic systems, this effect cannot be observed unless the dimensions of the structures are in the nanometer regime. The reason for this different behaviour is the small spatial dimension of the space charge regions due to the effective screening of the induced charges by the conduction electrons.

In nanoporous metals and thin films exposed to appropriate electrolytes, it has been demonstrated that substantial changes of physical properties can be induced by the application of a potential between the nanostructured metal and a counter electrode. Examples of the changes of surface stresses and the electrical resistivity of thin Gold films [1] and nanoporous Gold [2] will be presented. A simple model is proposed based on the modification of the electron density distribution at the interface of the metal and the electrolyte. Effectively, the corresponding change of the effective thickness of the sample is the major cause of the observed resistivity change.

Additionally, a transparent conducting oxide, ITO, in a nanoparticulate form has been prepared from a dispersion using spin coating. The observed resistivity changes, i.e. the on/off ratio can be as large as 2.000, i.e. 200.000 %, between the different values of the control potential [3]. Moreover, the device exhibits field effect transistor behavior identical to a conventional semiconductor, but in this case observed in a material with a large charge carrier density exhibiting metallic conductivity. The ITO dispersion can be deposited using established ink-jet techniques to prepare printable electronic devices. Additionally, the mobility is approx. 25 cm²/Vs, i.e. much larger than most organic printable devices and, moreover, stable at ambient conditions. Studies of the tuneability of the conductivity, scanning tunnelling microscopy and spectroscopy in ITO thin films with various thicknesses have been used to understand the origin of the large changes of conductivity in these nanomaterials.

References:

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- [3] S. Dasgupta, S. Gottschalk, R. Kruk, H. Hahn, *Electrochemically-gated field-effect transistor with Indium Tin Oxide nanoparticles as active layer*. Nanotechnology (2008). **19**: 435203.

PL.S.II.2

MULTILAYER COATINGS FOR X-RAY OPTICS

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Periodic and aperiodic multilayer coatings consisting of ultrathin bilayers on the nanometer scale are essential components of X-ray optics for advanced X-ray analytical equipment and for synchrotron beam lines. Typical examples are filters of small or large spectral bandwidth, components for shaping high-intensity X-ray beams with highest reflectivities, or mirrors for light sources with an active optical length of more than 1 meter. Their functionality is based on X-ray scattering from alternating amorphous layers of materials with large differences in atomic number. Modern thin film deposition technologies allow to fabricate such multilayer systems with reproducible control of layer thickness and resulting excellent reflectivity properties. The development of those layer systems requires precise monitoring of layer thickness, layer periodicity and uniformity, and of interface quality on different length scales. Transmission electron microscopy (TEM) of multilayer cross-sections enables analysing the decisive structure parameters which is essential for controlling the layer deposition and assessing the X-ray reflectivity properties. We have used high-angle annular dark-field scanning TEM and high-resolution TEM imaging of multilayer cross-sections, combined with numerical analyses of digitized image intensity profiles, such as the geometric phase analysis, and show that high precision can be achieved in determining quantitative values for the local layer dimension and interface roughness. Comparisons for different multilayer coatings on silicon substrates show good agreement with nominal deposition parameters and with thickness values derived from spatially averaging X-ray reflectivity measurements.

The contributions of the colleagues and the co-authors on the related publications are gratefully acknowledged. Funding by the ISH Innovationsstiftung Schleswig-Holstein (contract HWT 2007-13 H) is gratefully acknowledged.

Keywords: multilayers, interfaces, sputter deposition, transmission electron microscopy, X-ray reflectivity.

PL.S.II.3

**POLAR OXIDE INTERFACES:
STRUCTURE AND COMPOSITION ON THE ATOMIC SCALE**

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When materials of different polarity meet at an interface, interface dipoles occur, which give rise to a diverging electric potential. For the case of $\text{LaAlO}_3/\text{SrTiO}_3$ it has been demonstrated, that this so called polar catastrophe is overcome by a charge transfer into the interface. In consequence, a two dimensional electron gas is established, which makes the interface between the two insulating materials conductive. In a similar way a conducting interface is expected for the $\text{DyScO}_3/\text{SrTiO}_3$ interface, since LaAlO_3 and DyScO_3 comprise the same polarity and are band insulators holding similar dielectric constants and energy gaps. However, our electrical measurements on $\text{DyScO}_3/\text{SrTiO}_3$ multilayers reveal insulating behaviour. High-resolution Z-contrast microscopy and electron energy loss spectroscopy are employed to measure the composition of individual atomic layers across the interfaces in a $\text{DyScO}_3/\text{SrTiO}_3$ multilayer system. An intermixing extending over two monolayers at the interfaces is observed for both, the Dy-Sr sublattice and the Sc-Ti sublattice. Furthermore, the valence of Ti is found to be constant throughout the layer system. Employing the ionic model the composition of the individual atomic layers can be translated into charges. Considering compensation between adjacent layers each of the layers is found to be neutral. Hence, the interfaces are expected to be insulating, which is confirmed by electric measurements. From this result it is concluded that in addition to charge accumulations, intermixing of cations can contribute to counteract the interface dipoles associated with the polar discontinuity.

PL.S.II.4

QUANTITATIVE NANOMECHANICAL TESTING IN A TEM

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Recent progress in both in situ and ex situ small-scale mechanical testing methods has greatly improved our understanding of mechanical size effects in volumes from a few nanometers to a few microns. Besides the important results related to the effect of size on the strength of small structures, the ability to systematically measure the mechanical properties of small volumes through mechanical probing allows us to test samples that cannot easily be processed in bulk form, such as a specific grain boundary or a single crystal. In the case of individual nanostructures, the need to address the nanostructure in a direct manner is even more acute, and in situ TEM in many cases makes this possible. This talk will demonstrate how individual nanostructures and individual microstructural features can be tested quantitatively inside a TEM with different loading schemes such as indentation, compression, and tension.

PL.S.II.5

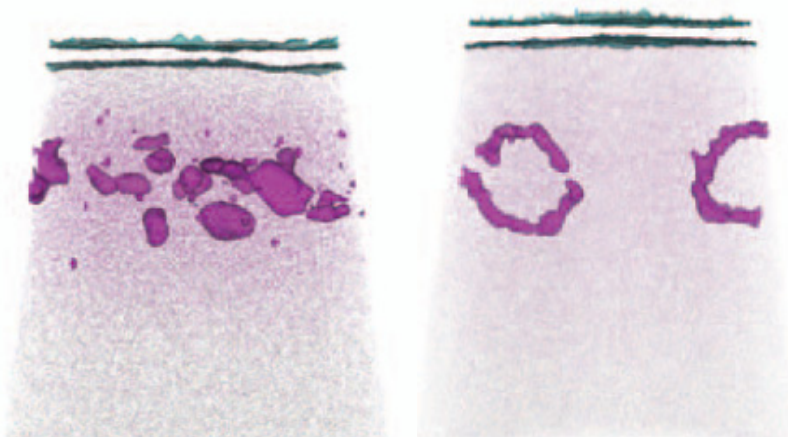
**PRESENT STATUS AND IMPORTANT NEW TRENDS
IN ATOM PROBE TOMOGRAPHY**

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Atom probe tomography (APT) provides three-dimensional structural and compositional analysis of materials at the atomic scale. Metals and alloys have been studied extensively by this technique for several decades. Recent specimen fabrication techniques using focused-ion beam instruments with in-situ manipulation have made it routine now to extract and analyze specimens from nanoscale structures including advanced alloys, device wafers and even finished components.

Major developments in atom probe technology by Cameca and Imago Scientific Instruments (now part of Cameca) including LEAP® and LAWATAP® have led to greater facility for running specimens and greater detail in quantitative analysis. These data are revealing important new information about processing effects and correlations with properties. The aim of this presentation is to review developments in instrumentation that have enabled major progress with applications. Examples will be given for a wide variety of materials including metals, semiconductors, ceramics, and even synthetic organics and polymers.



APT image of arsenic dopants (purple) implanted into silicon.

(Left) Cluster defects after rapid thermal anneal at 600°C. (Right) Vacancy dislocation loops after drive-in anneal at 1000°C. Purple isoconcentration surfaces are shown for arsenic at 2 at%. Blue feature is an isoconcentration surface for oxygen which delineates the native oxide at the top of the images. From: K. Thompson, Philip L. Flaitz, Paul Ronsheim, David J. Larson, and Thomas F. Kelly, *Science* 317 (2007) 1370.

PL.S.II.6

**THE USE OF MeV IONS FOR SECONDARY ION MASS SPECTROMETRY
WITH SIMULTANEOUS PIXE AND RBS**

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For more than 30 years the sputtering of large molecules from molecular solids using high energy (MeV) heavy primary ions has been a topic of interest. The technique was initially termed "Plasma Desorption Mass Spectrometry" (PDMS) and it utilized the high energy density deposited into the electronic system by fast heavy ions to create high sputtering yields of secondary ions. These secondary ions can be extracted from the target and analyzed in a time-of-flight secondary ion mass spectrometer (ToF-SIMS) to gain molecular information of the surface material. We report here on how this technique has been developed using a typical Oxford Microsystems microprobe system to allow molecular maps of surfaces to be produced. Typically beams of 10MeV O^{4+} have been used, which also allow simultaneous PIXE and RBS elemental maps to be taken. It is also possible to allow the beam to exit the vacuum system and to perform these experiments at (or near) atmospheric pressure. This novel experimental setup will be described and some applications of the system will be presented.

The process for molecular ejection from a molecular solid via this process is not well understood, but the MeV ion is expected to break the bonds of the molecules along the ion track as it penetrates the material. Thus it is expected that this technique will only be good for molecular imaging below the static limit – where the ion does not re-sample an area that has been affected by a previous ion. However, recent results, using the system for forensics applications, have demonstrated an unexpected apparent ability to obtain depth profile information from the sputtered molecular solid. Further experiments and simulations on multilayer molecular solids have been made to determine how this might be possible and these will be reported here.

PL.S.II.7

FIRST-PRINCIPLES STUDIES ON TRADITIONAL AND EMERGING MATERIALS

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Quantum-mechanical first-principles calculations are well established as explanatory and, in cases, predictive tools of modern materials science and applied physics. Here I will discuss distinct examples of density-functional theory ab initio simulations of key properties in materials of technological importance. First, I will present results which enable us to understand basic features of interfaces encountered in today's electronic devices. In particular, I will discuss issues related to the morphology and defect properties of the boundaries between Si or Ge substrates and gate dielectrics in electronic transistors. The migration of impurities in diffusion barrier materials, such as transition-metal nitrides, employed in devices or as hard coatings, will cover the second part of talk. Finally, I will address a number of defect-related processes in graphene and carbon nanotubes (CNT). These processes unravel the atomic-scale mechanisms of self-healing in graphitic nano-systems and of phenomena present in CNT-based nanoelectromechanical devices.

PL.S.II.8

**MECHANISMS OF DYNAMIC VOID GROWTH BY DISLOCATION EMISSION
FOR NANO AND MICRON SIZE VOIDS**

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The image force exerted on a nearby dislocation by the free surface of a circular void is evaluated, for a dislocation emitted from the surface of the void, and for a dislocation that has arrived near void by glide from the remote distances. This analysis is used to study the growth of nanovoids and micron size voids. Among all directions available for dislocation emission from the surface of the void, the direction of the most likely emission is determined. The critical stress and the direction of the dislocation emission are determined for the voids under remote uniaxial, pure shear, and arbitrary biaxial loading. The analysis includes ledge effects and the effects of the loading orientation relative to the discrete slip plane orientation. It is shown that dislocations are emitted more readily from larger nanovoids and that dislocations with a wider dislocation core are emitted under lower applied stress than dislocations with a narrow dislocation core. The growth of micron size voids takes place by different mechanisms and under much lower stress than what is required for the growth of nanovoids.

O.S.C.1

**CHARACTERIZATION OF INTERFACES
IN A MODEL CERAMIC-METAL SYSTEM**

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Despite efforts to characterize ceramic-metal interfaces, the understanding of such structures lags far behind that of bulk constituents. The detailed study of a model system – platinum in sapphire (single crystal alumina) – was motivated by the relative dearth of information on the structure of metal-oxide interfaces. Platinum nano-precipitates (<100nm diameter) were formed in sapphire by high-energy ion implantation followed by thermal annealing in air. Processing parameters anticipated to yield a large number of precipitates with a high symmetry orientation relationship were used to produce the specimens and these specimens were used for detailed characterization of precipitate morphology and interfacial structure. Platinum precipitates in sapphire that had been annealed at 1600°C in air were imaged with the TEAM 0.5 microscope at the National Center for Electron Microscopy. Atomic-resolution phase-contrast images of the sapphire-Pt interfaces were produced and exit wave reconstructions of through-focal series were compared to simulated images to extract quantitative information about structure and bonding at the interfaces. Conventional and high-resolution transmission electron microscopy were used to characterize the morphology of precipitates after annealing for 100h at 1600°C. The information derived from the high-resolution imaging of the interfaces will be related to the quantitative description of the precipitate morphology. This research was supported by the Metals & Metallic Nanostructures Program of the National Science Foundation through Grant No. 080506. This work performed, in part, under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The assistance of the staff at the National Center for Electron Microscopy is gratefully acknowledged.

O.S.C.2

SYNTHESIS OF ZnO-C NANOCOMPOSITE USING FUSED SALT ELECTROLYSIS

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Zinc Oxide-Carbon composites have been considered as interesting active materials for electrochemical supercapacitors. In this paper, for the first time, synthesis of ZnO-C nanocomposite by electrolysis of fused LiCl-ZnCl₂ using graphite cathode will be discussed. Product comprising of carbon -surrounded ZnO nanoparticles were characterized by using of high resolution SEM, EDX ,DSC and BET analyses.

Keywords: ZnO, carbon, nanocomposite, electrolysis, fused salt.

O.S.C.3

STRUCTURAL AND LUMINESCENCE STUDY OF In AND Fe DOPED ZnO NANOWIRES AND NANORIBBONS

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Indium and iron doped ZnO nanowires, nanoribbons and other nanostructures have been grown by a thermal vapor-solid method. The starting material was a mixture of ZnS or ZnO powders and powder of the dopant oxide. Nanoribbons of indium doped ZnO, often curved with ring shape, were obtained. Indium incorporates either in the ZnO nanostructures or leads to the formation of nanoribbons of the indium-zinc-oxide compound Zn₄In₂O₇. Luminescence of the nanoribbons has been studied by time resolved cathodoluminescence (CL) in SEM. Fe doped ZnO nanowires are obtained by the same method. The influence of Fe doping on the defect structure and the optical behavior of the nanowires was investigated by CL.

O.S.C.4

MICROSTRUCTURE AND CATALYTIC PROPERTIES OF OXIDE THIN FILMS DEPOSITED BY PLD TECHNIQUE

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In this paper the results of the investigations of Cu and Nd doped CeO₂ and SnO₂ thin films deposited by PLD technique are presented. These thin films could exhibit metallic or semiconducting properties. The general interest in these systems is based firstly on their applications as electrodes that are stable at high temperatures, and secondly, on catalytic interactions with specific gases (methane, carbon monoxide, etc.). The main interest in these composite systems is associated with their variable catalytic responses in the presence of CO-containing gases, as well as their conductivity.

The study was carried out using different parameters of process (substrate temperature, laser beam energy). The structure, chemical composition, phase composition and morphology of obtained surface layers was examined (SEM, TEM, HREM, EDS, XRD, AFM).

The laser energy, the substrate temperature and the oxygen pressure in the vacuum chamber during deposition by PLD process influence strongly chemical composition microstructure and morphology of obtained thin films. Research showed that Cu doped CeO₂ thin films shows good catalytic responses in the presence of CH₄.

Keywords: thin films, pulsed laser deposition, Cu and Nd doped CeO₂ and SnO₂ oxides, catalytic properties.

O.S.C.5

DIFFRACTION FROM MS2 NANOTUBES

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Symmetry of quasi-one dimensional regular systems gives their classification into 15 infinite elementary conformation classes. Expression for diffraction intensity and characteristic features of the diffraction patterns are found for each of these classes [1]. Nanotubes and various nanowires are composed of one or more configuration classes, which allow direct application of the results. In particular, MS2 (M=Mo,W) nanotubes are considered. Possible characterization of the tubes (chirality and number of walls) is discussed.

[1] T. Vukovic, I. Milosevic, and M. Damnjanovic, Physical Review B **79** (2009) 165439

O.S.C.6

COILED SINGLE-WALL CARBON NANOTUBES

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More than fifteen years have passed since the first report of experimental evidence of regularly coiled carbon nanotubes [1], but, the structure, formation mechanism and theoretical aspects of these nanotubes still remain unresolved [2].

We propose model of hexagonal, helically coiled single wall carbon nanotubes, determine their line group symmetry [3] and calculate electronic band structure of the relaxed configurations by means of fully symmetry adopted density functional tight binding method implemented into the *POLSym* code [4]. Electrical properties of the straight and coiled carbon nanotubes of different chiralities are compared and analyzed.

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O.S.C.7

INTER-LANDAU LEVEL SCATTERING PROCESSES IN MAGNETIC FIELD ASSISTED THz QUANTUM CASCADE LASER

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We present a detailed analysis of GaAs/AlGaAs terahertz quantum cascade laser (QCL) in the presence of an intense external magnetic field. One of the objectives in further development of THz QCL is the realization of structures operating at higher temperatures. This is difficult to obtain as the operating photon emission energy is smaller than the longitudinal-optical (LO) phonon energy in the semiconductor material. With increased temperature, electrons in the upper radiative state gain sufficient in-plane energy to emit an LO-phonon, which represents a non-radiative scattering and reduces the optical gain. By applying strong magnetic field, two-dimensional continuous energy subbands become split into series of discrete Landau levels, and at particular values of B it is possible to quench these non-radiative channels. Numerical simulations are performed on two-well design quantum cascade laser operating at 4.6 THz, implemented in GaAs/Al_{0.15}Ga_{0.85}As, and the magnetic field is perpendicular to the epitaxial layers. Strong oscillations of carrier lifetimes for the upper state of the laser transition, as a function of magnetic field, are observed. These can be attributed to interface roughness scattering and LO phonon scattering between Landau levels, with two different contributions to each individual scattering mechanism.

O.S.C.8

**INFLUENCE OF THE NANOSTRUCTURE ON THE SURFACE
AND BULK PHYSICAL PROPERTIES OF MATERIALS**

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Fullerenes, nanotubes, quantum dots have been considered as effective sensitizers to modify both the spectral, optical, nonlinear optical features, dynamic and polarization characteristics, as well as mechanical properties of the organic and inorganic materials. Laser, spectroscopy, mass-spectroscopy, nuclear magnetic resonance methods have been apply to support the change in the physical properties of the new nanocomposites. The extending of the nanocomposites applications area has been considered.

O.S.C.9

ALUMINOPHOSPHATE-BASED CHABAZITE AS A NANO-OXIDE CARRIER

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²*Jožef Štefan Institute, Ljubljana, Slovenia*

Chabazite is one of the most widespread natural zeolites. Also, it is one of the first zeolites to be studied as an ion-exchanger. The aluminosilicate network is a nanoporous three-dimensional framework with ellipsoidal apertures having dimensions of about 0.37x0.42 nm, which classifies the chabazite as a molecular sieve with small pore openings. At the beginning of the 1990's, very extensive research in the field of zeolite synthesis led to the discovery of novel compounds with zeolite structures. Among them, porous aluminophosphates are the most important class. The zeolite-like aluminophosphates can be synthesized hydrothermally in the presence of various organics which play a structure-directing role. Here we report the main structural characteristics of the chabazite-like aluminophosphate obtained in the presence of *tris*(diaminoethane)nickel(II) complex. Upon crystallization the complex, nickel(II) ion exhibits not only the templating role in connecting and arranging the tetrahedral AlO₄ and PO₄ structural units but also plays a co-structuring role. By losing one ethylenediamine ligand from its coordination sphere upon hydrothermal crystallization, Ni(II) ion forms an unseal P-O-Ni-O-P bridge across the chabazite cage. The encapsulation of the Ni(II) complex inside the lattice leads to a deformation of chabazite-like lattice. Thermal treatment of the as-synthesized material led to decomposition of the Ni(II) complex. HRTEM analysis of the calcined product shows that it contains an aluminophosphate-based chabazite and a nickel oxide phase. Nickel oxide is present in the form of spherical nanocrystalline particles homogeneously dispersed in the chabazite matrix. The sizes of the oxide crystallites are between 2-7 nm, with the average particle measuring ~ 5 nm in diameter. The SAED pattern recorded over multiple nickel oxide particles corresponds to the cubic NiO structure (i.e. JCPDF # 78-0643). This work shows that amine complexes of Ni(II) can serve as useful templates for the crystallization of nanoporous aluminophosphates and that the thermal decomposition of the complexes captured inside the aluminophosphate host can be a suitable method for obtaining fine nano-oxide particles.

O.S.C.10

**NOVEL POLYCARBONATE-BASED POLYURETHANE ELASTOMERS,
PREPARATION AND CHARACTERIZATION**

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Polycarbonate-based polyurethane (PC-PU) elastomers were prepared by one-step technique. Polycarbonate diols (of M_w 1000 or 2000, kindly provided by Asahi Kasei Chemical Corporation) were used as soft-segment-domain component; and hard domains of PC-PU consist of 1,6-hexamethylene diisocyanate and 1,4-butanediol (chain extender) products. Either dibutyltin dilaurate (0.05 wt. %) or even no catalyst were used in the procedure. Some samples also contained layered nanoparticles (Bentonite for organic systems). The main characterization of PC-PU is aimed mainly on measurement of mechanical properties (tensile characteristics and dynamic mechanical thermal analysis). Tensile properties of all products are excellent: very high elongation at break together with good tensile strength lead to excellent toughness (expressed at the energy necessary to break the sample per volume unit). Glass transition temperature of soft segments was about -32 °C for all samples. Atomic force microscopy (AFM) was used for determination of 'bulk' properties of PC-PU (surface analysis of fracture areas of samples broken prior the analysis).

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O.S.C.11

**LASER ELECTRODISPERSION FABRICATION OF NANOPATTERNS
FOR SER(R)S OPERANDO SPECTROSCOPY**

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In this paper we report on the application of laser electrodispersion (LE) to deposit amorphous gold nanoparticles (AuNPs) with a narrow size distribution on the Si and SiO_x surfaces. The particles were deposited on etched and oxidized Si wafers and studied by TEM, SEM and XPS. Their application in surface enhanced Raman spectroscopy (SERS) is described using methylene blue and crystal violet as target molecules. The AuNPs proved to be efficient to detect very low concentrations of analytes (10^{-8} M). Further, AuNPs were deposited into microchannels etched in silicon wafers. The channels were closed with glass using anodic bonding and commercial adhesives. The suitability of these systems to be used as continuous-flow SERS for operando spectroscopy was studied.

O.S.C.12

**SYNTHESIS OF MESOPOROUS TITANIA FILMS TEMPLATED
BY NOVEL AMPHIPHILIC TRIBLOCK COPOLYMER PEO-PB-PEO**

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Control over the pore structure of mesoporous materials is a key factor for tuning their functionality in applications such as catalysis, adsorption and biotechnology. Such control is gained employing micelles of amphiphilic block-copolymers as pore templates. We report the synthesis of a series of novel template molecules poly(ethylene oxid)-*b*-poly(butadiene)-*b*-poly(ethylene oxid) (PEO-PB-PEO) that extends the size range of templated mesopores towards bigger pores than achieved with typical commercial block-copolymers. The polymers were used to prepare mesoporous nanocrystalline TiO₂ coatings of different pore size. Remarkably, the polymer templates controlled mesoporosity not only with common molecular precursors (TiCl₄), but also using titania nanoparticles as building blocks. SAXS, TEM, SEM and BET analysis reveals the influence of choice of polymer and precursor on pore structure, pore ordering and film shrinkage during thermal treatment.

O.S.C.13

CHARGE MEMORY EFFECTS IN InN NANODOTS

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Charge memory effects and hysteresis loops of I-V curves in InN semiconductive nanodomains are demonstrated by using conductive atomic force microscopy. The memory effects originate from large accretion of surface charges either at the interface between the crystal and the amorphous phase of InN, or from the reflection of Bloch wavefunctions at the surface of a single InN nanocrystal due to boundary conditions. The charges were confined within a 0.3 nm thin surface layer from the interface. The total charge at the boundary depends linearly on the size of nanocrystals. The InN nanostructures are synthesized by pulse laser deposition at 157 nm on Si substrates.

O.S.C.14

NANOSIZE WO₃ FOR GAS SENSING AND PHOTOCATALYSIS

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For applications in gas sensors, catalysis, photoelectrochromical cells and chromogenic devices, tungsten oxides have attracted much attention in the past decades. Tungsten oxide has several polymorph. We searched the relationship between the morphology, the composition and the properties. We studied the tungsten oxides on several applications (gas sensing, photocatalysis). Samples were prepared through annealing hexagonal ammonium tungsten bronze. These samples were analyzed by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy, solid state ¹H-MAS NMR and X-ray photoelectron (XPS) spectroscopy, UV-VIS reflectance spectroscopy. By varying the heating temperature, we could control the crystalline structure, while by adjusting the annealing atmosphere, we managed to control the average oxidation state of the samples. Then, we studied tungsten oxides as gas sensors, as photocatalysts (in aquas –and gas phase too). It was found that both the crystalline structure and the composition had strong influence on the gas sensitivity and catalytic activity

O.S.D.1

**SOME ASPECTS OF PROCESSING AND PROPERTIES
OF COMPOSITE MATERIAL WITH Si-C PARTICLES**

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Composite materials are defined as materials consisting of two or more components with individual characteristics and whose combination leading to synergistic effects that lead to new applications in different phases of the components considered separately.

The manufacturing technology of metal matrix composites reinforced with particles are still in the attention of researchers worldwide because of interest shown in the modernization and optimization of current technologies and improving the properties of composite materials and their effectiveness in use. Using a Taguchi experimental plane, applied manufacturing technology which has the objective function of the composite mechanical properties have been identified optimal values of the factors with significant influence. The experimental results on mechanical properties were analyzed by further investigations on the structure of composites, fracture and defects identifiable by ultrasonic testing of composite material particles ranfort Si-C, distribution of C, Si and others elements along the reference line, microhardness, tensile tests results of base alloy and composite material obtained and diffractometers determinations.

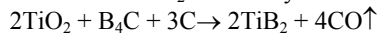
O.S.D.2

**MICROSTRUCTURE –MECHANICAL PROPERTIES RELATIONS
IN PRESSURELESS SINTERED SiC-TiB₂ COMPOSITE**

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Densification and mechanical properties (fracture toughness, flexural strength and hardness) of SiC-TiB₂ composite were studied. Pressureless sintering experiments were carried out on samples containing 0 to 50 vol% of TiB₂ created by in-situ reaction:



Al₂O₃ and Y₂O₃ were used as sintering additives to create liquid phase and promote densification at sintering temperature of 1940°C. The sintered samples were subsequently heat treated at 1970°C. It was found that the presence of TiB₂ serves as an effective obstacle to crack propagation thus increasing both strength and fracture toughness of sintered SiC-TiB₂ composite. The subsequent heat treatment of sintered samples promoted elongation of SiC matrix and improved mechanical properties. The optimum volume fraction of TiB₂ ranged from 12 to 24 vol%. Typical microstructures of samples with the mentioned volume fractions of TiB₂ consist of TiB₂ particles (< 5µm) uniformly dispersed in a matrix of elongated SiC plates. The maximum flexural strength of 593 MPa was obtained in samples with 12 vol% TiB₂ whereas the maximum fracture toughness of 6.6 MPam^{1/2} was measured in samples containing 24 vol% TiB₂. The relations between microstructure and mechanical properties were discussed.

O.S.D.3

**STUDY OF FORMATION AND MESOSTRUCTURE OF YTTRIUM
HYDROXOCARBONATE MONODISPERSE SPHERICAL PARTICLES**

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Though large body of works dedicated to the synthesis of various compounds by hydrolysis in presence of urea is produced, the mechanism of monodisperse particles formation and especially influence of synthetic parameters on their morphology yet requires to be studied. This is the question not only of scientific interest but also of great practical importance as application of such materials in luminescent devices puts very strict limitations on their morphological parameters including shape, size and size distribution of particles. Thus the main goal of this work was to study the influence of major synthetic parameters, including concentration of reagents, temperature and duration of hydrolysis process, surface tension and ionic strength of initial solutions, on mesostructure, shape, size, and size distribution of forming particles of $Y(OH)CO_3 \cdot xH_2O$. It was shown that variation of such parameters as pH and concentration of reagents allows to control morphology and size distribution of precipitated particles as well as their surface condition and mesostructure. The work was supported by RFBR (grants # 10-03-01187, 09-03-12191-ofi-m and 09-03-01067).

O.S.D.4

**METAL-MATRIX COMPOSITES DISPERSION-STRENGTHENED BY
NANOPARTICLES FOR DIAMOND TOOLS APPLICATION**

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Cu-, Co-, and Fe- based metal matrix composites (MMCs) produced by powder technology are seeing wide use as a matrix for diamond-containing composites employed in cutting, drilling, grinding applications, etc. The cutting ability of diamond segments is known to depend markedly on the mechanical, physicochemical, and tribological properties of the matrix material (binder). Severe service conditions (intense hydroabrasive wear, impact stresses, and elevated temperature in the cutting area) demand that the mechanical and tribological properties of binders be improved. Development of new MMCs reinforced with nanoparticles is a promising way to resolve the problem. The use of nanosized particles (instead of microsized ones) for reinforcement of hard compounds is advantageous for the following reasons. According to the Orowan equation, the effectiveness of dispersion strengthening depends on the particle size of embedded particulates, so that a relatively low amount of reinforcing phase (below 5 vol %) can be expected to markedly improve the mechanical, physicochemical, and tribological properties of reinforced alloys. The chemical activity of nanoparticles is known to be higher than that of bulk material due to better interparticle contact between the components. Interaction between the nanoparticles and diamond grains also improves the adhesion of binder to diamond crystal and hence the tool life time. In this work, we have investigated the effect of nanosized powders WC, ZrO₂, C_{nt} (carbon nanotubes) and others additives on the properties of sintered dispersion-strengthened Cu-, Co-, and Fe-based MMCs. Starting mixtures were prepared in a centrifugal planetary mill under controllable balls/mixture ratio and varied treatment duration. The sintering kinetics was found to depend on whether or not the interaction between added nanoparticles and matrix powder takes place (using as examples inactive ZrO₂ and reactive WC nanoparticles). An increase in the amount of added nanoparticles leads to their aggregation and accumulation of conglomerates in the porous interparticle space of the binder, which exerts a decelerating effect on the compaction process. In hot-pressed samples, the reinforcing phase was found both in the grain body and its boundary. Dispersion-strengthened MMCs produced by hot pressing technology showed an increase in the hardness (by 5–10 HRB), bending strength (by 54%), wear resistance (by a factor of 2–10) and a decrease in the friction coefficient. The use of designed alloys as a binder of diamond tools for cutting reinforced concrete gave a 2-fold increment in the service life of tools, without reduction in their cutting speed.

O.S.D.5

**TRIBOLOGICAL PROPERTIES OF Si_3N_4 + SiC AND Al_2O_3 + SiC
NANOCOMPOSITES**

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The influence of the sintering additives (La_2O_3 , Y_2O_3 , Yb_2O_3 and Lu_2O_3 in Si_3N_4 + SiC) and SiC addition (from 2 to 20 vol% in Al_2O_3 + SiC) on the microstructure and tribological behavior of Si_3N_4 + SiC and Al_2O_3 + SiC nanocomposites has been investigated. Ball on disc method has been used for the wear test at room and high temperatures. FE SEM, TEM, HREM and AFM have been used for the microstructure characterization and for the study of the wear mechanisms. The composites exhibited finer microstructure compared to monolithic materials and the aspect ratio of the Si_3N_4 grains increased with decreasing ionic radius of rare-earth elements both in monolithic Si_3N_4 and in Si_3N_4 +SiC nanocomposites. The interrelationship between the microstructure and wear characteristics has been described.

O.S.D.6

**PROCESSING TECHNOLOGIES FOR DISCONTINUOUSLY REINFORCED
LIGHT METALS**

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Discontinuously, which means particle, short fiber and in-situ reinforced light metals can be attractive alternatives to very high performing, but also very high priced continuous fiber reinforced metal matrix composites (MMC). However, application relevant properties of reinforced light metals strongly depend on their processing, which is again dependent on the nature of the reinforcement phase (geometry, chemistry). Therefore, existing processing techniques are discussed with respect to the final composite properties and cost. Possible applications are derived from the range of mechanical properties that can be manufactured. Alternative processing routes and new material compositions are described, aiming on excellent mechanical properties at ambient cost for an increase in the application fields of reinforced light metals.

O.S.D.7

**MANUFACTURING OF CONTINUOUS FIBER REINFORCED LIGHT METAL
MATRIX COMPOSITES BY THERMAL SPRAYING OF PREPREGS**

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Due to their excellent mechanical and physical properties fiber reinforced Light Metal Matrix Composites (LMMC) are promising candidates which can be used in high performance parts in the automotive and aerospace industry. The production of fiber reinforced metals with conventional manufacturing techniques like squeeze casting or diffusion bonding leads to restrictions in the component's geometry and results in elevated manufacturing costs. The potential of metal matrix composites can be increased by applying new, fast and cost-effective manufacturing technologies. With this aim, the manufacturing method by thermal spraying of matrix material on fiber substrates and subsequent densification and shaping to the final composite component was developed. For cost-effective coating and reduced thermal load on sensitive fiber substrates, the industrially well-established twin wire electric arc spraying technique is used for material deposition. Most applications require a well-defined orientation of the reinforcement therefore the fiber-orientation should be customized to 2D or even complex 3D multi-directional fiber structures. The introduced technology for MMC manufacturing allows the flexible processing of these tailored fiber structures. The paper also comprises results in term of microstructure and mechanical properties of the composites with different types of fibers.

O.S.D.8

LOCK-IN IR THERMOGRAPHY METHOD FOR EVALUATION OF LIGHT COMPOSITE ARMOURS

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Light composite armour is a preferred solution against military and paramilitary sources of present threats as the reducing mass of battle vehicles provides a possibility of their quick air-transport. The light armours of these vehicles should be resistant against:

- common and rifle bullets,
- grenades,
- anti-personal mines,
- IED – improvised explosive devices.

The composites reinforced by fibres are used in structural elements of vehicle trunks. Materials of composite armours include graphite epoxy, glass epoxy and aramid fiber composites. The composites that have been examined can include a variety of defects, such as ballistic impacts, embedded defects, manufacturing defects, thermal damage, moisture ingress and other induced defects.

Methods for testing ballistic protection of light armours are known and used. First of all they consist of checking armours resistance against the bullets where the bullet velocity is known. Moreover the V_{50} velocity is defined during the test. In this method the V_{50} velocity of a round or standard fragment is defined (according to STANAG 2920) as the velocity at which armour is penetrated at the probability 50%. The distribution of points hit by bullets or fragments on the surface of an armour is also important. In fact, only correct distribution of these points provides a guaranty for an impartial assessment of tested designs. After hitting by a bullet, shape and size of an area of damage in composite armours depends on the type and design of armour, and type of reinforcing material is particularly important. Knowledge of damage characteristics allows arranging hitting points to avoid overlapping of damaged areas. Considering quality and protection ability of armour, the extent of internal damage should be kept in mind except the direct ability to stop bullets and fragments. The Military Institute of Armament Technology in cooperation with Military Institute of Armour & Automotive Technology carried out a project on using nondestructive testing method in order to evaluate destruction zones in a light ballistic armour which appear as a result of impact of bullets and fragments.

Nondestructive testing by using active lock-in IR thermography method is very useful in evaluation of internal defects. In the paper we present the dependence between the energy of fragments/or bullets and the dimension of internal defects.

O.S.D.9

**SPIN-DEPENDENT MAGNETORESISTANCE AND MAGNETIZATION
IN OXIDIZED FeCoZr-AL₂O₃ GRANULAR NANOCOMPOSITES
WITH «CORE-SHELL» STRUCTURE**

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Formation of «core-shell» in granular nanocomposites (GNCs) containing superparamagnetic (SP) metallic nanogranules in dielectric matrix leads to the enhanced spin-dependent tunneling magnetoresistance (MR) due to the interface effects and size distribution of cores and shells. Present study is focused on the correlation between temperature T and magnetic field B dependencies of MR and magnetization M of the oxidized GNC (FeCoZr) _{X} (Al₂O₃)_{100- X} films with «core-shell» structure. Granular nanocomposite films (FeCoZr) _{X} (Al₂O₃)_{100- X} (26 at. % $\leq X \leq 69$ at. %), sintered by ion-beam sputtering of complex target in oxygen-free ($P_{Ar} = 6,7 \cdot 10^{-2}$ Pa) and oxygen-containing ($P_{Ar+O} = 9,6 \cdot 10^{-2}$ Pa, $P_O = 4,2 \cdot 10^{-3}$ Pa) sputtering ambient onto glass-ceramic substrate were the object of investigation. Magnetization of samples $M(B)$ was studied by Quantum Design VSM-PPMS setup in the temperature range $T_{mes} = 4,2 - 300$ K in magnetic fields B up to 8,9 T. Temperature dependencies of magnetization $M(T)$ were measured in field-cooled (FC, $B = 50$ Oe) and zero field-cooled (ZFC) regimes. MR of the samples was measured by four-probe method in closed-cycle cryostat in the temperature range $T_{mes} = 4,2 - 300$ K in magnetic fields B up to 8,0 T. ⁵⁷Fe Mössbauer spectroscopy in the temperature range 77-300 K was applied for phase composition analysis. «Core-shell» structures, containing SP FeCoZr granules covered with complex (Fe³⁺)Co-oxide - (Fe²⁺)Co-oxide shell and SP (Fe³⁺)Co-oxide core encapsulated inside paramagnetic (Fe²⁺)Co-oxide shell were assumed basing on transmission Mössbauer spectroscopy data for (FeCoZr)₃₅(Al₂O₃)₆₅ and (FeCoZr)₅₉(Al₂O₃)₄₁ films, respectively. Temperature dependent magnetometry of the oxidized GNC films revealed decreased M_S values, unsaturated character of $M(B)$ curves at temperatures 2-3 K and some peculiarities of $M(B)$ recorded in FC-ZFC regimes confirming the formation of structure like «ferromagnetic FeCoZr core - (Fe³⁺)Co, (Fe²⁺)Co oxide shell». Reasonable coincidence of MR and squared normalized magnetization $-(M/M_S)^2$ reveals spin-dependent tunneling originating from «core-shell» structure. Enhanced spin-dependent tunneling in «core-shell» structures for all studied films compositions should be considered within the frame of the assumption of spin-filter role of (Fe³⁺)Co, (Fe²⁺)Co oxide shells. No traces of exchange AFM-FM coupling between FeCoZr core and (Fe³⁺)Co, (Fe²⁺)Co oxide shell was detected at low concentration of metallic nanoparticles in GNCs containing fully isolated «core-shell» nanogranules. Enhanced coercive force H_C in GNC film at low temperatures is assigned to the pinning effect of nanogranules spins within the interface between FeCoZr-(Fe³⁺)Co, (Fe²⁺)Co, or (Fe³⁺)Co, (Fe²⁺)Co-Al₂O₃ independently on the magnetic nature of these interfaces.

O.S.D.10

**NANOCOMPOSITE MATERIALS BASED ON FLUORITE OXIDES AND Ni/YSZ:
SYNTHESIS, PROPERTIES AND CATALYTIC PERFORMANCE IN STEAM
REFORMING OF CH₄ AND BIOFUELS**

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Nanocomposite materials comprised of Ni/YSZ (20-90 wt.%) combined with doped Ce-Zr oxides and promoted by Pt or Ru were synthesized via Pechini and (co)impregnation routes. The samples were characterized by BET, XRD, TEM and H₂ TPR. The catalytic properties of the nanocomposites were studied in the steam reforming (SR) of methane, ethanol and acetone at short contact times in stoichiometric feeds. Some correlations of catalytic performance with the surface/lattice oxygen mobility/reactivity, Ru (Pt) and NiO dispersion changed due to the dopant nature and content have been established. Performance of best compositions supported as porous strongly adhering layers on Ni/YSZ anode cermets or crofer/fechraloy porous monolithic substrates was demonstrated to be also high and stable for all types of fuels ensuring reformat composition close to equilibrium.

O.S.D.11

**A STUDY ON DELAMINATION-FREE DRILLING
OF CARBON FIBRE REINFORCED PLASTICS**

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Carbon fibre reinforced plastics are increasingly being used in automotive and aerospace industries, mainly because of their particular properties. In the aerospace industry, drilling operations are the most frequent because of the need to obtain holes for riveting and fastening screw assemblies of structures. However, problems arising from drilling, namely the damage induced can lead to the rejection of a significant number of components. This paper presents some results of a possible approach to damage-free drilling of carbon fibre reinforced plastics (CFRP). Design of Experiments and Surface Response Methodology were used to obtain empirical models to quantify the drilling damage.

O.S.D.12

**PREPARATION AND OPTIMALIZATION OF SILICON OXYCARBIDE
COMPOSITES TOUGHENED BY INORGANIC FIBERS BY PYROLYSIS
OF PRECURSOR COMPOSITES WITH SILOXANE MATRIX**

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In this contribution, the preparation of silicon oxycarbide composites with inorganic fibers is described. The main focus of this contribution is on the synthesis of the oxycarbide matrix. The preparation procedure consists of a well-controlled sol-gel reaction of alkylated alkoxy silanes which are first converted to soluble oligomeric branched siloxane resins. These resins, which easily impregnate fibrous materials, are subsequently cured to hard highly polymeric siloxane thermoset networks. The final preparation step is the pyrolysis of the siloxane precursor to silicon oxycarbide and gaseous by-products. In this work, we focused on the optimization of the composition of the oligomeric precursor resin, especially on changing the silicon-carbon ratio (monomers with different alkoxy functionality and alkyl groups) and on varying the degree of oligomerisation. The effects of the tested liquid resin precursor modifications on the curing and on the subsequent pyrolysis are compared. The mechanical and fracture properties of the best matrix samples are discussed, as well as of fibrous composites based on them.

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O.S.D.13

**PHASE RELATIONS AND ADVANCED MATERIALS
IN THE CeO₂-Ln₂O₃ SYSTEMS**

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Doped ceria is an important material in view of its potential applications as a solid electrolyte for its use in oxygen sensors and in solid oxide fuel cells. It is also a candidate material for application in controlling air-to-fuel ratio in automobile exhaust. In addition, ceria finds its application in optical polishing, petroleum cracking catalyst, nuclear reactors components etc. Phase equilibria in these systems are important for the development of advanced ceramics.

Present work is about phase equilibria in the binary systems CeO₂-Ln₂O₃ (Ln= La, Sm, Gd, Er) at 600-1500 °C in air in the whole concentration range. X-ray diffraction, petrography and electron microprobe X-ray diffraction were used to determine phase contents. The microstructures of the sintered ceramic samples were examined by using the scanning electron microscopy (SEM). The boundaries of the phase fields were determined. The lattice parameters of the unit cell for solid solutions were refined.

The phase relations in CeO₂-La₂O₃, CeO₂-Sm₂O₃, CeO₂-Gd₂O₃ and CeO₂-Er₂O₃ systems have been established at 600-1500 °C. The phase relations differ as the CeO₂-La₂O₃ system showed only two single-phase regions, namely hexagonal (A) and cubic with fluorite-type structure (F) solid solutions based on lanthana and ceria are in equilibrium at 1500-1100 °C. The ceria solubility in hexagonal lanthana is around 25 mol % and 15 mol %, respectively. The lanthana solubility in the F-CeO₂ was found to be around 49 mol %. Whereas CeO₂-Sm₂O₃ and CeO₂-Gd₂O₃ systems showed three single-phase regions, namely monoclinic (B), cubic form of rare-earth oxides (C-type) and cubic (F-type) solid solutions based on samaria, gadolinia and ceria are in equilibrium at 1500 °C, which are divided by two phase fields (F+C) and (B+C). The stabilization of C-type rare-earth oxides after Ce⁴⁺ substitution, which is attributed to decrease in average cationic size on Ce⁴⁺ substitution at Ln³⁺ site were observed.

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Keywords: ceria, rare-earth oxides, lanthana, samaria, gadolinia, erbia, phase equilibria, solid solutions, lattice parameters, fluorite, ceramic functional materials, structural materials.

O.S.D.14

**PROCESSING OF INTEGRAL SKIN CELLULAR POLYMERIC COMPOSITES
IN RAPID ROTATIONAL FOAM MOLDING**

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The conventional rotational molding process has evolved over the years into a technology that allows for creating a polymeric cellular reinforcing structure, i.e., a distinct foamed layer or core within the interior of hollow moldings that can be encapsulated entirely within a solid skin integrated boundary layer thereby forming integral-skin cellular polymeric composites. However, the production of integral skin cellular polymeric composites using the conventional rotational foam molding process suffers from undesirably lengthy processing cycle times, high energy-intensiveness, and the lack of efficient means for real-time process control during both the heating and cooling segments of the cycle. In addition, previously conducted research indicated credible evidence of a strong counter-proportional causality between the duration of the rotational molding cycle and the quality of the obtained cellular morphologies. This paper introduces Rapid Rotational Foam Molding, 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. This processing approach provides advantageous potentials for the manufacture of advanced multi-layered single-piece cellular composites with uniform skin wall thicknesses while reducing the processing cycle time and the energy consumption to a fraction of previous common levels.

PL.S.III.1

**CROSS-LINKING BEHAVIOR IN GELATIN – HYDROXYAPATITE
NANOCOMPOSITE**

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Development of cross-linking in a nanocomposite comprising gelatin (GLT) and hydroxyapatite (HAp: $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) was elucidated. Nanocomposite sols were prepared *via* an in situ precipitation route, whereby HAp / GLT ratio was systematically varied and the relationship between the properties of the composites before and after gelation was examined. HAp particles were needle-like with significant chemical interaction with GLT matrices. As the GLT concentration was increased, the crystallinity of HAp decreased with increasing extent of lattice distortion along a-axis. B-type carbonate substitution predominated in the samples of GLT concentration above 50%, presumably due to lattice distortion. Sedimentation did not occur at GLT concentration above 60% with well-developed cross-linked networking. The interaction between HAp and GLT and the GLT intermolecular cross-linking are associated with the carbonyl interaction of GLT with a critical value. Three exothermic peaks were observed on DTA at around 330°C, 360°C, and 420°C. They are associated with different types of GLT intermolecular interaction, *i.e.*, those among random coil, critical nucleus, and triple helix structure. High HAp concentration disturbs GLT to form cross-link bonding and decreased the Vickers hardness of the composites after gelation. The strong GLT crosslink in sol was preserved after gelation. Thus, it is possible to predict the formation of GLT network in gel from the properties of corresponding sol.

PL.S.III.2

MIMICKING THE GENESIS OF TOOTH ENAMEL

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In the following respects, tooth enamel is a unique tissue in the mammalian body: (a) it is the hardest tissue in it; (b) its microstructure is dominated by parallel rods composed of bundles of 40 – 60 nm wide apatite crystals with the aspect ratios reaching up to 1:10,000; c) it is the most mineralized tissue in the mammalian body, comprising 96 - 98 wt% of the mineral phase; and (d) not only does the protein matrix that gives rise to enamel guides the crystal growth, but it also conducts its own degradation and removal in parallel. To satisfy the latter requirement while mimicking the process of amelogenesis in vitro, the three aspects of the process are promoted and investigated in their synergy: (a) crystal growth; (b) protein assembly; and (c) proteolytic digestion. Experimental settings based on controlled and programmable titration of amelogenin sols with buffered calcium and phosphate solutions were employed to imitate the formation of elongated enamel-like crystals.

Dynamic light scattering and zeta-potential analyses were performed to discern the most optimal conditions for the protein-mineral interactions that foster the uniaxial crystal growth, while atomic force and scanning electron microscopies were utilized during characterization of the crystallization process, in addition to different elemental analyses. The following are the main conclusions that will be pointed out in this presentation: (a) despite its predominantly hydrophobic nature, amelogenin acts as a promoter of nucleation and crystal growth under experimental conditions applied in this study; (b) the apatite morphologies obtained at pH 6.5 show higher levels of semblance with respect to its biological counterpart in enamel when compared to those obtained at pH 7.4; (c) proteolysis exerts an additional nucleation- and growth-promoting effect; (d) constant titration rate settings with the initial supersaturation ratio equal to zero prove as particularly convenient for the controlled, epitaxial growth of apatite.

PL.S.III.3

ELECTRON ENERGY-LOSS SPECTROSCOPY (EELS) FOR NANOPLASMONIC APPLICATIONS IN MATERIALS SCIENCE

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The optical properties of metallic nanoparticles are dominated by plasmon resonances, which are oscillations of the conduction electrons when the nanoparticles are coupled to the electromagnetic field. By controlling the geometry and material of the nanostructure and its surrounding medium, one can tailor its plasmon resonant modes for applications such as optical wave-guiding, surface-enhanced Raman spectroscopy and single-molecule detection. A scanning transmission electron microscope (STEM) equipped with an electron energy-loss (EEL) spectrometer and monochromator is a powerful method to study surface plasmons in noble metallic nanostructures because of its high spatial (~ 1 nm) and energy (~ 0.2 eV) resolution. This paper describes the use of monochromated STEM-EELS techniques to probe localized surface plasmons in chemically synthesized silver nanoparticles and silica/gold core-shell particles. In silver nanoparticles dimers, the plasmon resonant modes are found to be highly dependent on the symmetry of the two interacting particles. For the gold/silica nanoparticles, the strength of the interaction between core and shell (defined by the difference in plasmon resonant modes) can be tuned by adjusting the relative ratio of core and shell dimensions. Efforts to accurately control nanostructure geometry for nanoplasmonic applications will also be discussed.

Funding for this work has been provided by the Engineering and Physical Sciences Research Council (EPSRC) in the UK.

PL.S.III.4

TAILORED IMPLANTS BY SELECTIVE ELECTRON BEAM MELTING

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In this contribution, the basic principles and opportunities of selective electron beam melting (SEBM) for load-bearing orthopedic applications are discussed. Selective electron beam melting, which belongs to the class of generative processes based on powder bed consolidation, offers a high potential for the production of tailored open-cellular metal implants for bone graft substitution. The porous structure not only promotes the fixation of the implant by bone ingrowth but is also a means to adapt the mechanical properties of the implant to the surrounding tissue.

As basis material we use pure titanium and the titanium alloy Ti-6Al-4V. The material consolidation process, the geometric resolution and particularly the surface roughness is illustrated and discussed with the help of numerical simulation. A diamond lattice structure is chosen to reveal the influence of the structure size and the relative density on the mechanical properties. Local tailoring of the mechanical properties of the implant is possible since the elastic modulus as well as the strength is governed by the relative density. The in vivo performance of a tailored implant is demonstrated in a sheep model.

PL.S.III.5

PLASMA TAILORED NANOSTRUCTURES AND THEIR ADVANCED APPLICATIONS

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The research on the growth of various nanostructure materials is intensifying in recent years, especially on application of reactive plasmas as a tool for fabrication. Nanostructures like nanowires (NW) are predominantly synthesized using catalyst clusters in either, the vapour phase, a supercritical fluid phase, a gas decomposition or by using an assisted growth technique without catalyst clusters. Another prominent method employed is bulk nucleation and growth of nanowires with plasma assisted growing from the melts of low-melting point material and also directly from the solid phase from bulk material. These solid phase procedures have been extensively reached by our group.

The subject of particular interest is application of low temperature reactive plasmas, also called chemically active plasmas, for direct plasma surface nanofabrication processes. These plasmas are mostly generated in high frequency discharges like microwave or radiofrequency discharges, where suitable radicals for nanofabrication can be generated. In presented cases, we used rf oxygen plasma glow discharge of weakly ionized highly dissociated plasma for nanostructuring various bulk metals.

On the surface of metals, metal oxide nanowires / nanocones / nanobelts / nanodots were grown during exposure to oxygen radicals. As simulations and experimental results show, the ionized gas environment is decisive in sustaining the growth of tall and sharp nanotips or nanowires. It is, however, not yet known, how the surface properties of a material change with the growth of nanostructures and the presence of other radicals. This becomes very important when we deal with reactive plasma process, where nanostructures like nanowires grow spontaneously from solid state material, so no building material is supplied from the gas phase. The growth of metal oxide nanostructures from bulk phase can be explained by of synergetic interaction of low energy ions and high flux of neutral oxygen atoms entering to the surface and changing its structural properties.

This new approach to nanostructuring metal surfaces by growing various nanostructures from solid state material by merely plasma radical interaction is opening new exciting possibilities of product manipulation in manufacturing process of microelectronic devices and gas sensors. With specific plasma parameters we can tailor shape, length, density or even a type of nanostructure grown on surface. The various cases will be presented.

PL.S.III.6

**NOVEL MECHANOCHEMICAL SYNTHESIS OF CARBON NANOMATERIALS BY A
HIGH-SPEED BALL-MILLING PROCESS**

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A novel mechanochemical approach inspired by the Allende meteorite to produce sophisticated carbon nanomaterials is reported. It is demonstrated that unique carbon nanostructures, including carbon nanotubes, carbon onions, and new carbon nanorings are synthesized by high-speed ball-milling of steel balls. The carbon nanorings have diameter of several ten nanometers. It is considered that the gas-phase reaction takes place around the surface of steel balls under local high temperatures induced by the collision energy in ball-milling process, which results in phase separated unique nano-carbon materials. This paper also report the mechanochemical synthesis of fine nanoparticles of Fe based complex oxide by the high-speed ball-milling process.

PL.S.IV.1

FROM HIGH TO LOW PERMITTIVITY GLASS-FREE MATERIALS FOR LTCC TECHNOLOGY

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In the last twenty years, a rapid development of various electronic devices (mobile phones, wireless local areas networks-WLAN, Bluetooth, etc.) for wireless communication has taken place. Such a progress led to the development of new materials and technologies, which enabled size reduction and increased functionality of various electronic components. Low Temperature Co-fired Ceramic (LTCC) technology has met the demands of miniaturization and integration by fabrication of 3-dimensional modules with integrated passive electronic components (capacitors, resistors and inductors). Because these modules are fired simultaneously, the development of a mechanically stable multichip LTCC structure having desired electrical performance requires the knowledge of chemical compatibility of the ceramics, their sintering behaviour as well as the dielectric and thermo-mechanical properties. This presentation elaborates the development of several glass-free LTCC materials in our Advanced Materials Department in the last two decades exhibiting a permittivity in the range from 5 to 90. In the first part of this presentation, an example of the combination of high and middle permittivity materials based on the system $\text{Bi}_2\text{O}_3\text{-Nb}_2\text{O}_5$, designed for the LC-filters is discussed. The multilayer structure of this LC-filter will be used as a model for exemplify the important issues related to the matching of materials in terms of their sintering behaviour and thermal expansion. The second part of this presentation will discuss the development of low-permittivity substrate LTCC materials. Because of the rigorous requirements for the electrical, mechanical and chemical properties, various materials have been studied. The first group of low-permittivity materials with promising dielectric properties ($\epsilon \sim 6$, $Q_{xf} > 100.000$ GHz, $\tau_f = -20$ ppm/ $^\circ\text{C}$) and sintering temperature $\sim 900^\circ\text{C}$ are based on gallogermanate-feldspars. In this respect, low price of the raw materials is often of high importance for practical applications. Thus, low permittivity materials based on the crystal structures of willemite (Zn_2SiO_4), scheelite, forsterite (Mg_2SiO_4) and wollastonite (CaSiO_3) were developed. Sintering at temperatures which meet the LTCC conditions was accomplished with additions of alkaline-earth oxides and/or zinc borates. The materials thus developed cover the whole range of thermal expansions coefficient (TCE) from 4-12 ppm/ $^\circ\text{C}$. Among these materials, willemite was used as a basis for the development of a low-permittivity material with low TCE (~ 4 ppm/ $^\circ\text{C}$), whereas a combination of scheelite and forsterite leads to a high TCE material (10-12 ppm/ $^\circ\text{C}$). Wollastonite based low-permittivity materials exhibited TCE of 5-7 ppm/ $^\circ\text{C}$. These materials exhibiting $\epsilon = 7-9$, $Q_{xf} = 20.000-70.000$ GHz and Ag-compatibility, are competitive with the commercially used glass-based LTCC materials.

Keywords: LTCC, glass-free, Ag-compatibility, high-low permittivity.

PL.S.IV.2

RECENT ADVANCES IN MAGNETIC NANOSTRUCTURES

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Nanostructured magnetic materials comprise a very active research field due to the new phenomena taking place at the nanoscale as a consequence of quantum, finite-size, surface and interfacial effects. In this talk, we will review some examples of these systems, focusing the attention on the phenomenology associated with the surface state in nanoparticles and exchange coupling between ferromagnetic (FM) and antiferromagnetic (AFM) layers. Magnetic nanoparticles are an excellent example of nanostructured materials, which provide the critical building blocks for the booming of many applications in nanotechnology. A key question in these systems is how the nanostructure modifies their magnetic and electronic properties. We studied 5 nm $\text{Fe}_{3-x}\text{O}_4$ nanoparticles, synthesized either by thermal decomposition of an iron organic precursor in an organic medium or coprecipitation of two iron salts in water. In the first case oleic acid was used as surfactant and was covalently bonded to the nanoparticle surface due to the high synthesis temperature; in the second case polyvinyl alcohol was used, leading to a protective coating but without any chemical bond. We showed through magnetic measurements and X-ray magnetic circular dichroism that covalently bonded nanoparticles displayed bulklike magnetic and electronic properties while nanoparticles with adsorbed coatings showed particlelike properties. The comprehensive explanation of the exchange bias phenomenon (EB) due to the exchange coupling between FM and AFM layers in nanostructured materials still remains a challenge, despite the number of experimental and theoretical investigations. In particular, EB could be a means to beat the superparamagnetic limit in ultrafine magnetic particles. In this talk, we report on the occurrence of EB in granular thin films composed of Co nanoparticles embedded in a Y-stabilized amorphous zirconia matrix, which were deposited by laser ablation. This method allows one to control the degree of oxidation of the Co particles just by tuning the oxygen pressure at the vacuum chamber during deposition. Consequently, we monitored the nature of the nanoparticles embedded in the nonmagnetic matrix from pure FM to pure AFM, with a FM/AFM intermediate regime for which the percentage of the AFM phase may be increased at the expense of the FM phase. We observed EB in partially oxidized particles as small as 2 nm. The mutual exchange coupling between the AFM and FM gives rise to the induced exchange anisotropy on the FM leading to high irreversible hysteresis loops, and the blocking of the AFM clusters due to proximity to the FM phase. We will also discuss our results about EB in ordered nanoelements nanofabricated on FM/AFM heterostructures. We used focused ion beam lithography to fabricate ordered arrays of square antidots on bilayered samples prepared by electron beam evaporation consisting of AFM FeF_2 (70nm) and FM Ni (50nm). We showed that the transition from positive to negative EB can be systematically tuned with antidot density. These results are a consequence of the energy balance and suggest that the nanostructure plays a key role in the formation of pinned uncompensated spin regions in the AFM layer. These *non* interfacial magnetic moments created at the antidot faces favor the onset of positive exchange bias at lower cooling fields. We have developed a model based on the micromagnetic simulations that allows accounting for all the foregoing results.

PL.S.IV.3

**CHARACTERIZATION OF MAGNETIC NANOCRYSTALS
FORMED BY MAGNETOTACTIC BACTERIA**

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Many organisms are known to contain ferrimagnetic nanocrystals, whose magnetic properties are determined by their sizes, morphologies, crystallographic orientations and arrangements. However, in most cases the relationship between the presence of the crystals and navigation by the organism in magnetic fields remains poorly understood. Magnetotactic bacteria are the simplest organisms that use magnetite (Fe₃O₄) or greigite (Fe₃S₄) crystals for orienting themselves in the Earth's magnetic field. We have used off-axis electron holography in the transmission electron microscope to characterize the magnetic fields of iron oxide and iron sulfide nanoparticles in magnetotactic bacteria in order to understand nanoparticle magnetism in the cells and to draw conclusions about possible mechanisms of magnetoreception in structurally more complex organisms.

We studied a variety of wild and cultured magnetotactic bacteria that contain magnetite nanocrystals of various sizes, shapes and arrangements, including single and double chains and disordered clusters. Electron holograms were used to construct magnetic induction maps, which showed that each crystal invariably contains a single magnetic domain and that in well-organized chains the magnetization directions of individual crystals are parallel to each other. Magnetic induction maps from magnetosomes with different sizes, morphologies, orientations and spacings suggest that shape anisotropy is the most important factor that controls the magnetic microstructure of chains of crystals, followed by interparticle interactions, with magnetocrystalline anisotropy being the least important. Some species of magnetotactic bacteria produce greigite magnetosomes. The morphologies and arrangements of iron sulfide magnetosomes are typically less strictly constrained than are those of magnetite magnetosomes, resulting in a lower magnetic moment per volume of magnetic material. The organism compensates for this reduced efficiency by synthesizing a correspondingly larger number of magnetosomes.

In all of the cells that were studied using electron holography, the magnetosomes were found to result collectively in a permanent magnetic dipole moment that is sufficient for effective alignment of the cell in the Earth's magnetic field.

PL.S.IV.4

BONDED INTERMETALLIC POWDERS FOR THE APPLICATION IN MAGNETIC REFRIGERATION

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Magnetocalorics (MC) are materials that show a magnetocaloric effect (MCE), which is defined as the heating or cooling of a magnetic material in response to the application of a magnetic field. Most magnetic materials exhibit a large MCE only at low temperatures, making them unsuitable for practical use in everyday life. But with the discovery of the giant MCE in $\text{Gd}_5\text{Si}_2\text{Ge}_2$ in 1997 by Pecharsky and Gschneidner¹, magnetic refrigeration (MR) became a viable and promising technology, which could become competitive with vapor cycle refrigeration. $\text{Gd}_5\text{Si}_2\text{Ge}_2$ is a ferromagnetic material with a spontaneous ordering temperature of 276 K. However, $\text{Gd}_5\text{Si}_2\text{Ge}_2$ magnetocaloric material as such cannot be used for practical application due to the high hysteresis losses. In 2004 Provenzano² reported a reduction of hysteresis losses in $\text{Gd}_5\text{Ge}_2\text{Si}_2$ by adding a small amount of iron to the alloy, forming $\text{Gd}_5\text{Ge}_{1.9}\text{Si}_2\text{Fe}_{0.1}$. The peak magnetic entropy change of the new material shifted from 275 K to 305 K, broadening its width, but reducing its value drastically. The purpose of our investigation was to find a compromise of both properties with a systematic study. We have investigated a wide range of Fe substitutions of the $\text{Gd}_5\text{Si}_2\text{Ge}_2$ magnetocaloric alloy with the aim to quantitatively clarify the effect of iron with respect to the reduction in entropy and hysteresis losses. Our activity was focused on substituting both elements (Si and Ge) with Fe ($\text{Gd}_5\text{Si}_{2-z}\text{Ge}_{2-z}\text{Fe}_z$). We were looking for a possible explanation for the interesting magnetic properties of the newly formed $\text{Gd}_5(\text{Si},\text{Ge})_3$ phase. With the addition of very small amounts of iron and substituting both Ge and Si atoms in basic alloy a *very high magnetocaloric effect was achieved, comparable to the one reported in previous papers, and with much lower hysteresis losses*. This material could be used in practical application as a bench material for construction of magnetic refrigerators. The goal was to fabricate the material in the shape of bonded sheets and/or discs. The critical problems to overcome are related to achieving the maximum packing density of the effective material and optimising the heat-transfer properties by the correct selection of bonding/binding material, and the dimensions of the sheets or discs. By selecting between various bonding materials the RT6000 resin was found to perform the right properties to fabricate 20 mm/2 mm discs so far.

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PL.S.IV.5

CRYSTAL STRUCTURE OF APATITE TYPE RARE-EARTH SILICATE $\text{SrLn}_4\text{Si}_3\text{O}_{13}$

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Apatites form a large family of compounds with general formula $\text{A}_{10}(\text{MO}_4)_6\text{O}_2$, where A can be an alkali, alkaline-earth, or rare-earth atom and M can be P, V, Si, B, or Ge. The reported space groups for most apatites include $P6_3/m$, $P6_3$, and $P2_1/m$. While the $\text{SrLn}_4\text{Si}_3\text{O}_{13}$ (Ln = La, Nd, and Y) apatite type rare-earth silicates have been well studied, most other rare-earth analogues have been largely ignored. In this work, the crystal structure of $\text{SrLn}_4\text{Si}_3\text{O}_{13}$ (Ln = La, Pr, Nd, Sm, Eu, Gd, Er, Tm, Yb, and Y) ceramics is examined. The ceramics have been prepared by the conventional solid-state processing route. Phase and structural analysis was carried out using powder x-ray diffraction and high resolution transmission electron microscopy. The crystal structure throughout the series was confirmed as hexagonal, with the space group of $P6_3/m$, via electron diffraction and refined via Rietveld refinement of x-ray diffraction data.

PL.S.IV.6

HYDROTHERMAL SYNTHESIS AND POST HEAT-TREATMENT OF $(\text{K,Na})\text{NbO}_3$ PARTICLES

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The effect of the starting molar ratio of KOH:NaOH on the crystal structure, chemical composition, and particle morphology of $(\text{K,Na})\text{NbO}_3$ (KNN) powders synthesized by a hydrothermal reaction at 220°C for 24 h was investigated. As the KOH:NaOH ratio in an alkaline solution with a total alkalinity of 10 mol/L was changed from 8.0:2.0 to 7.0:3.0, the phase of the synthesized KNN powders changed from K-rich KNN single phase to Na-rich KNN single phase, via two-phase mixtures consisting of K-rich KNN and Na-rich KNN. The two-phase mixed KNN powders were transformed into single-phase KNN powders by post heat-treatment at 850°C for 5 h in air. Inductively coupled plasma (ICP) analysis revealed that KNN powders with an average K:Na ratio of 1:1 could be synthesized when the KOH:NaOH ratio was around 7.35:2.65. The particle morphology of the synthesized KNN powders was also influenced by the KOH:NaOH ratio.

O.S.E.1

**HIGH-VELOCITY SUSPENSION FLAME SPRAYED (HVSFS) BIOACTIVE
HYDROXYAPATITE COATINGS**

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Hydroxyapatite (HAp) coatings are widely used for various biomedical applications due to the fact that HAp is a bioactive, osteoconductive material capable of forming a direct and firm biological fixation with surrounding bone tissue. Bioceramic coatings based on nanoscale HAp suspension were thermally sprayed on Ti plates by high-velocity suspension flame spraying (HVSFS). HVSFS is a novel thermal spray process, developed at IMTCCC, for direct processing of submicron and nano-sized particles dispersed in a liquid feedstock. The deposited coatings were mechanically characterized. The adhesion strength of the layer composites were analyzed by the pull-off method and compared for different spray techniques. The coatings and initial feedstock were analyzed using X-ray diffraction (XRD), micro Raman spectroscopy and scanning electron microscopy (SEM). Rheology analysis was performed for the HAp suspension. The coating composites were also immersed in simulated body fluid (SBF) to indicate bioactivity.

O.S.E.2

**NANO-BIORESORBABLE POLYMER SPHERES AS CARRIERS
FOR TRANSDERMAL DELIVERY OF KETOPROFENE**

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The transdermal delivery system provides a highly efficient, safe, and easy to use method for delivering active ingredients and other compounds to the body through intact skin, thereby offering many other advantages over the traditional dosage forms. Ketoprofen is a poorly water-soluble non-steroidal antiinflammatory drug and widely used for the acute and long-term treatment of rheumatoid arthritis and associated diseases.

The purpose of the study presented in this paper has been to examine the possibility of the synthesis of a new nanoparticulate system for drug delivery of ketoprofen suitable for transdermal applications. Multi-scale design of a transdermal drug delivery system, from the molecular or nano scale through the macroscopic scale, was analyzed.

The obtained nano particles contain ketoprofen-loaded spheres of poly(D,L-lactide acid) (PDLLA). Characterization was performed with wide-angle X-ray structural analysis (XRD), infrared spectroscopy (FT-IR), field-emission scanning electron microscopy (FESEM), high performance liquid chromatography (HPLC) and particle sized distribution (PSD) methods. XRD and FT-IR analyses confirmed that the ketoprofen is immobilized into PDLLA. The encapsulation of ketoprofen into the PDLLA nanoparticles was highly accomplished and the drug loading efficiency was 75%. The observed average particle dimension (d₅₀) of ketoprofen-loaded nano particles was 63 nm.

O.S.E.3

**PLGA NANOSPHERES AS DRUG CARRIERS FOR WATER- SOLUBLE VITAMINS:
IN VITRO AND IN VIVO STUDIES**

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Polymer materials like copolymer poly(DL-lactide-co-glycolide) (PLGA), due of their biodegradable and biocompatible nature, are widely used in various medical applications; controlled release of delivering drugs, carriers in the tissue engineering, fixation of the bone fractures, surgical strings, etc.. PLGA nanospheres in the size range 90-150 nm were produced using physicochemical method with solvent/non-solvent systems. The encapsulation of the ascorbic acid in the polymer matrix was performed by homogenization of water and organic phases. *In vitro* degradation and release tests of PLGA nanoparticles without and with encapsulated ascorbic acid were studied for more than sixty days in PBS and it has been determined that PLGA completely degrades within this period fully releasing all encapsulated ascorbic acid. The cytotoxicity of PLGA and PLGA/ascorbic acid 85/15% nanoparticles was examined with human hepatoma cell lines (HepG2 ECACC), *in vitro*. The biodistribution of ^{99m}Tc-labeled PLGA particles without and with encapsulated ascorbic acid after the different periods of time of their instillation into rats was examined. The radioactivity was measured by an (NaI) γ counter. The samples were characterized by X-ray diffraction, scanning electron microscopy, stereological analysis, transmission electron microscopy and ultraviolet spectroscopy.

O.S.E.4

**SONOCHEMICAL SYNTHESIS OF SILVER NANOPARTICLES AND
SILVER/HYDROXYAPATITE NANOCOMPOSITES**

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Concerning the recent intensive development of large number of variations of pathogens and their resistance to currently available anti-inflammatory pharmaceuticals, noble metals are one of the most promising antibacterial and antiviral agents today. However there is a need for a careful design of these nanomaterials in order to estimate desired outcome required for the future practical application which is an urgent condition for nowadays nanotechnology development.

In this work, sonochemical precipitation method was optimized for formation of nanosized silver particles and nanostructured hydroxyapatite/silver biocomposite. Different silver precursors able to be complexed with urea were applied and after the thermal decomposition of resulted silver-complex, nanosized metallic silver particles were obtained. As a result, different morphological properties of silver and silver/hydroxyapatite particles as a function of the silver source were obtained. Depends on the type of precursor, metallic silver particles were up to 10 nm in size randomly distributed over the surface of hydroxyapatite rods or up to 30 nm with axial organization onto the hydroxyapatite plates. Reaction mechanisms of formation of these structures and mechanism of their growth are investigated.

Silver has ability to diffuse from its composites or coatings therefore an achieving a stability of its particles is a required condition for its application in the field of nanomedicine. For that reason stability of metallic silver within silver/hydroxyapatite composite was investigated under two different pH of the medium during the period of ten days in order to determine concentration of released silver ions and to obtain preliminary data about possibility of concentration-related toxic effect.

O.S.E.5

**THE INVESTIGATION OF PERIODONTAL LIGAMENT CELL GROWTH
ONTO WATER/O₂ PLASMA TREATED PCL SUBSTRATES**

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In this contribution, low pressure water/O₂ plasma assisted treatment was applied in order to obtain COOH functionalities on the surface of 2D, poly-ε-caprolactone (PCL) substrates. Plasma treatment of PCL substrates was performed in a cylindrical, capacitively coupled RF-plasma-reactor in three steps: H₂O/O₂-plasma treatment; in situ (oxalyl chloride vapors) gas/solid reaction to convert –OH functionalities into –COCl groups; and hydrolysis for final COOH functionalities. DoE (Design of Experiment) software program was used for the optimization of plasma modification. COOH/OH functionalities on modified surfaces were detected quantitatively by using fluorescent labeling technique and UVX 300G sensor. Electron spectroscopy for chemical analysis (ESCA) was used to evaluate the relative surface atomic compositions and the carbon and oxygen linkages located in non-equivalent atomic positions of untreated and modified surfaces. Atomic force microscope (AFM) analysis showed that nanoscale features of the PCL surfaces are dramatically changed during the surface treatments. Periodontal ligament (PDL) fibroblasts were used in cell culture studies. Cell proliferation was assessed by MTT (3-[4,5-dimethylthiazol-2-yl]-diphenyltetrazolium bromide) analysis. Confocal Laser Scanning Microscopy (CLSM) was used for determination of cellular morphology and cytoskeleton organization. Cell culture results showed that plasma treated 2D PCL substrates were favorable for the PDL cell spreading, growth and viability due to the presence of functional groups and/or nanotopographies on their surfaces.

O.S.E.6

**EPIDERMAL LAYERS CHARACTERISATION
BY OPTO-MAGNETIC FINGERPRINT**

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According to most literature data, the skin is usually observed as a simple structure with equivalent electrical model, which include general properties of epidermis, basal membrane and dermis. In this paper, we analyzed the skin structure as a more complex system. Particularly we analyzed epidermis from layers approach and its water organization in nano ordered sublayers. Using opto-magnetic fingerprint (OMF) method, which is very sensitive to paramagnetic/diamagnetic properties of tissue, we found out that lipid-water structure ordering in layers play very important role in skin properties.

We investigate human epidermis properties for two different types of drinking waters, normal (N) and on edge to be normal (Z). We use fifteen volunteers who have been drinking Z water for years and five people who are drinking N water. For all of them we characterized surface of skin by OMF, then we remove *stratum corneum* by sticking plaster and characterized first layer of *stratum granulosum* by OMF, than we removed *first* half of *stratum granulosum* and characterized it, and *finally* we removed second half part of *stratum granulosum* and characterized the first layer of *stratum spinosum*. From day of experiment to next six weeks ten volunteers who drank Z water, start to drink N water. After eight weeks we make epidermis characterization by OMF. Five people who are drinking N water and five people who are drinking Z water become control group.

In our initial investigation we are found out difference of skin properties of people who change from Z to N drinking water. The significant difference posses middle part of *stratum granulosum*, where water-lipid sublayers exist. These preliminary results indicate impotence of water nanolayers presence in epidermis and type of drinking water for human skin properties.

O.S.E.7

**HYDROPHOBIC-HYDROPHILIC INTERACTIONS IN PROTEIN FOLDING,
PROTEIN-PROTEIN ASSOCIATION AND MOLECULAR RECOGNITION***

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Many biochemical processes such as protein folding or self assembly of proteins are highly specific. Proteins fold spontaneously into a very specific 3-dimensional structure. Proteins also associate spontaneously to form multi-subunit macromolecules. These processes occur in aqueous media. The question we pose is what is the role of water in these processes?

Until recently it was believed that the hydrophobic effect, i.e. the tendency of hydrophobic groups to "escape" from the aqueous environment is the dominant driving force for these processes.

Analysis of all the solvent induced contributions to the thermodynamic driving forces for protein folding and protein-protein association reveals that, contrary to the commonly accepted paradigm, hydrophilic interactions might be more important than hydrophobic interactions.

This conclusion was reached after critically examining the data on the various contributions to the driving forces for protein folding, and protein-protein association. Examples on the role of hydrophilic interactions on solubility of proteins, protein folding, protein-protein association and molecular recognition will be presented. Thus, hydrophilic interactions not only helps in understanding the role of water in biochemical processes, but they can also be applies to design drugs that bind stronger to their targets.

O.S.E.8

LIQUID CRYSTALLINE WATER AND THE LIVING STATE

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The remarkable properties of protoplasm, the stuff of living cells and organisms, have been noted since the beginning of the 19th century. Soon afterwards, water was recognized as a 'bound' constituent of protoplasm and the unusual properties of such 'bound' biological water became the focus of enquiry.

However, it was not until Gilbert Ling's Association-Induction (AI) hypothesis (Ling, 1962, 1984) that the pivotal role of water in living organization became explicitly defined. The AI hypothesis proposes that the major components of living protoplasm – water, proteins, and K^+ - exist in a closely associated, high-energy state.

In my laboratory, we discovered that living cells and organisms are highly coherent, dynamic, liquid crystalline phases; and furthermore, the large amounts of associated water, both within the cells and in the extracellular matrix, are an integral part of the organisms' liquid crystalline living state (Ho, 1993, 1998, 2008; Ho *et al.*, 2006).

There has been a great deal of progress in water research within the past decade. I shall review some key findings in support of a theory of the living state in which liquid crystalline water plays the leading role.

Poster Presentation

P.S.A.1.

ALUMINIDE FORMATION BY SPARK ALLOYING OF METALLIC SUBSTRATE

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The spark alloying enables transfer of metallic material from the electrode into substrate. Due pulsed spark the heat transfer into substrate is limited. Despite that diffusion bonding of material from electrode with material of substrate is possible, assisted also with exothermic reaction between components that forms aluminide. Presented are results of light microscopy and EDS analyses of in situ formed nonstoichiometric Fe-aluminides. The benefit of the aluminide on the surface of metallic substrate is formation of Al₂O₃ protective layer that increases the resistance to oxidation and in case of Fe-aluminide also resistance to sulphidation.

P.S.A.2.

PREPARATION AND CHARACTERISATION OF MAGHEMITE-CM-DEXTRAN FERROFLUID FOR THE APPLICATION IN MAGNETIC HYPERTHERMIA

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In the last decade magnetic nanoparticles as a material become very important in technological and biomedical applications. Maghemite superparamagnetic nanoparticles are non-toxic (biocompatible) and may serve as colloidal heating mediators for magnetic hyperthermia, when they are exposed to an external AC magnetic field. The heating effect of maghemite superparamagnetic nanoparticles exposed to AC magnetic field is governed by the mechanisms of magnetic energy dissipation. Magnetic ferrofluid (MF) was prepared from maghemite superparamagnetic nanoparticles coated with CM-dextran and dispersed in water. Nanoparticles were synthesized by alkaline coprecipitation from the aqueous solution containing Fe²⁺ and Fe³⁺ ions. After coprecipitation nanoparticles were coated with CM-dextran using a sonicator and ultrafiltrated in order to remove the excess of unbonded surfactant. Size and morphology of the magnetic nanoparticles were determined using transmission electron microscopy (TEM), while crystal structure was identified by X-ray diffraction. The amount of CM-dextran adsorbed on the magnetic particles was determined using the thermal gravimetric analysis (TGA) and the magnetization of the samples was measured using a Quantum Design SQUID magnetometer. Specific absorption rate (SAR) of the aqueous magnetic ferrofluid was determined with calorimetric measurements at 100 kHz and magnetic field strengths with amplitude up to 3.7 kA/m. Dynamic light scattering (DLS) was used to determine the hydrodynamic radii of maghemite nanoparticles coated with CM-dextran.

P.S.A.3.

SYNTHESIS OF COPPER-NICKEL NANOPARTICLES PREPARED BY MECHANICAL MILLING OR MICROEMULSION METHOD

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A physical or chemical method has been applied for the preparation of copper-nickel alloy particles in nanometric range. The particles were designed to be used for controlled magnetic hyperthermia applications.

Cu_xNi_{1-x} materials were prepared by mechanical milling and microemulsion method. The milling conditions were optimized using the desired alloy composition. Utilizing a ball-to powder mass ratio of 2, we can obtain nanocrystalline Cu_{27.5} Ni_{72.5} (at %) alloy with crystallite size around 10 nm and the Curie temperature of 45 °C.

Microemulsions with Ni²⁺ and Cu²⁺ salts were prepared using n-heptane/SDS/butanol /H₂O system. The nanoparticles with a desired composition were obtained after reduction of their salts with N₂H₄ and heat treatment in a tube furnace in Ar-H₂ atmosphere at 500 °C.

Thermal demagnetization in the vicinity of the Curie temperature of nanoparticles was studied by modified TGA-SDTA method. The morphology and size of particles was determined with XRD measurements and TEM analysis. Their magnetic properties were also investigated with VSM magnetometer.

P.S.A.4.

SYNTHESIS AND CHARACTERIZATION OF Cu-Ni MAGNETIC NANOPARTICLES FOR HYPERTHERMIA APPLICATIONS

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The copper-nickel alloys are being used in engineering, metallurgical industries because they have good magnetic, electronic and catalytic properties. In the last years, they have found increasing interest in biomedical applications. In this paper, we investigated structural and magnetic properties of copper-nickel alloys with respect to the applications for hyperthermia.

We prepared copper-nickel alloys with different compositions and methods. The first method was a physical, in which nickel powder and copper powder were mixed in different compositions, which were elaborated by high-energy milling. The mixture was ball milled for 20 hours to obtain a highly homogenous composition. In the second method we prepared alloys using microemulsions of SDS/n-butanol/n-heptane/water at 70°C under Ar/H₂ atmosphere. The products were heat treated in tube furnace for 5 h at 500°C in Ar/H₂ atmosphere.

The Cu-Ni alloy nanoparticles were characterized using X-ray diffraction (XRD) analysis, transmission electron microscopy (TEM) and the magnetometry. The Curie temperature for alloy particles was also measured with modified TGA-SDTA method.

P.S.A.5.

**DEPENDENCE OF SURFACE AND ZETA POTENTIALS OF SILICA ON pH IN
AQUEOUS ELECTROLYTE SOLUTIONS**

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Surface potential (ψ_0) of silica was calculated from the potentiometric acid-base titration data. The site-binding (s-b) model for the determination of electrical double layer properties of hydrous oxides was applied. Silica sol prepared from a sodium silicate solution by the ion exchange method was used. Various concentrations of monovalent electrolytes were used in titration. The dependence of surface potential on pH is linear and slightly dependent on the electrolyte concentration. The obtained slopes varied from 25 to 40 mV/pH for all investigated electrolytes and pH values (6.5 to 9.5). These values are lower than the value expected from the Nernst equation (60 mV/pH).

Zeta potential (ξ) measurements of silica were performed using a Zeta-sizer nano ZS apparatus equipped with MPT-2 Autotitrator (Malvern Instruments, UK), at various concentrations of potassium nitrate, at 25⁰C. Zeta potential, for all investigated electrolyte concentrations (0.001-0.10 mol.dm⁻³), increased from -30 mv to - 5 mv for pH values from 8.5 to 2.0, respectively. No Iso Electric Point (IEP) of the silica sample, at investigated experimental conditions, was obtained.

P.S.A.6.

**NON-ISOTHERMAL THERMOGRAVIMETRIC STUDY
OF CuO REDUCTION BY HYDROGEN**

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The reduction of commercial (Merck p.a.), (C) and synthesized (S), copper (II) oxide to metallic copper was studied by thermogravimetry under non-isothermal conditions. The gel-combustion technique was used to prepare S sample. The particles of both sample types were non-uniform in size with almost spherical morphology. The XRD analysis evidenced that the structure of C sample corresponded to CuO. Reduction process was carried out under flow of gaseous Ar + 25% H₂ mixture. Initial values of activation energy was estimated by Kissinger method and the results obtained were 64.95 kJ/mol (C) and 60.20 kJ/mol (S). The dependence of activation energy on the conversion degree (α) was studied by means of both isoconversional Friedman and multi-heating rate Coats-Redfern method. A more complete approach to the determination of the kinetics parameters (E_a , preexponential factor (A), reaction order (n) and parameter m) was done by means of two-parameter (m, n) autocatalytic model (Šesták-Berggren equation) which was found to describe in the best way the process under investigation ($A=4.597 \cdot 10^4 \text{ s}^{-1}$, $E_a=61.37$ kJ/mol, $m=0.653$ and $n=0.873$ for *S sample*, $A=1,430 \cdot 10^4 \text{ s}^{-1}$, $E_a=64.41$ kJ/mol, $m=0,677$ and $n=0,832$ for *C sample*). Particle size of the metallic particles obtained upon reduction depended on the type of sample and on the heating regime during reduction.

P.S.A.7.

MICROEMULSION-MEDIATED HYDROTHERMAL SYNTHESIS OF LiFePO_4 CATHODE MATERIAL

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LiFePO_4 is a material of great interest as cathode material for lithium ion batteries thanks to its good characteristics. One of the advanced techniques for LiFePO_4 powder preparation is hydrothermal synthesis. In this work, LiFePO_4 powders were prepared by a new approach, a microemulsion-mediated hydrothermal method in which microemulsion medium was further treated by hydrothermal reaction. The main advantage of the proposed route is low reaction temperature and short processing time that prevents agglomeration in the formed particles. LiFePO_4 powders were prepared by microemulsion-mediated hydrothermal method in cyclohexane/Triton X-100/n-hexanole/water at 180 °C. The product of hydrothermal synthesis was heat treated in reductive atmosphere to avoid oxidation of Fe^{2+} to Fe^{3+} . Powders were characterized by X-ray diffraction, scanning electron microscopy and galvanostatic charge-discharge cycling.

P.S.A.8.

SAMARIUM-DOPED CERIA THIN FILMS ON FTO GLASS OBTAINED BY ELECTRODEPOSITION

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Ceria-based oxides have been extensively used as oxygen ion conductors in solid oxide fuel cells, gas sensors, catalytic supports or promoters for automotive exhaust gas conversion reaction, glass polishing materials, ultraviolet absorbers. In particular, much attention has been focused recently on the preparation of rare earth ions-doped CeO_2 for enhancing its electrical, optical, magnetic or catalytic properties.

This work reports on pure ceria and Sm-doped ceria (SDC) thin films, deposited potentiostatically onto F-doped tin oxide (FTO)-coated glass substrates, from nitrate solution at room temperature. The as-grown films and films annealed at different temperatures were characterized by means of X-ray diffraction, scanning electron microscopy, energy dispersive X-ray, Raman and ultra visible spectroscopies. It was shown that samarium addition into electrolytic solution influences the electrodeposition process and induces changes in the structural, optical and morphological properties of the obtained ceria films. Effect of annealing temperature was studied and discussed as well.

P.S.A.9.

**NANOCOMPOSITES $Y_2O_3:RE@SiO_2$ AND $Gd_2O_3:RE@SiO_2$:
MICROWAVE SYNTHESIS AND LUMINESCENT PROPERTIES**

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Nanocomposites consisting of optically transparent glass or polymer matrix with luminescent nanoparticles dispersed in its volume are promising materials for chemical sensors, nonlinear-optic devices and first of all high-performance lasers. Earlier we've established that most effective is distribution of particles which size is times smaller than wavelength of excited radiation in transparent dielectric matrix. Thus the aim of present work was to develop technologically simple method of microwave sol-gel synthesis of luminescent nanocomposites based on uniformly distributed in transparent amorphous SiO_2 matrix particles of Y_2O_3 and Gd_2O_3 doped with rare-earth ions. We've studied relations between particles composition, size, uniformity of their distribution in matrix on one hand and luminescent properties of synthesized composites on the other. The work was supported by RFBR (grants # 09-03-12191-ofi-m and 09-03-01067).

P.S.A.10.

**PARTICLES FORMATION DURING PULSE PLASMA NITRIDING
AND a-CN_x:H COATING DEPOSITION ON HOT WORK STEEL SAMPLES**

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Generation of particles during combined diffusion/deposition process of hydrogenated carbon nitride film formation in DC pulse plasma was investigated. Plasma enhanced chemical vapor deposition (PECVD) is frequently employed for a-CN_x:H film deposition, but in our experiments a continuous diffusion/deposition treatment was applied. During diffusion processing the samples made of hot work steel grade H11 were nitrided at various pulse plasma parameters. Following plasma nitriding a carbon containing gas was introduced in process chamber which resulted in transition from diffusion to deposition processing mode. The electrically conductive spherical particles of different size were formed onto deposited hydrogenated carbonitride films and were partially incorporated in the coating. The origin and grows of spherical particles was discussed comparing the results of some rf and pulse plasma surface treatment. The experiments demonstrated possibility of a continuous diffusion/deposition pulse plasma processing intended for tribological applications. The influence of the nitrogen content in nitrogen-hydrogen plasma, substrate temperature, treatment time, pulse duty cycle and frequency on diffusion and compound zone formation was investigated. The obtained surface structures were characterized by the optical microscopy, microhardness measurements, calotest method, Raman and IR spectroscopy, XRD analyses and SEM microscopy

Keywords: Pulse plasma nitriding, a-CN_x:H coating deposition, continuous diffusion deposition, dust particles formation, hot work steel.

P.S.A.11.

THE INFLUENCE OF CHEMICAL TREATMENT OF CARBON MONOLITH ON SILVER DEPOSITION

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Carbon monolith (CM) was treated in order to obtain the samples with different oxygen complexes at the surface. The chemical treatment involved submerging the as-received CM in HNO₃, KOH and H₂O₂ solution. Silver deposition at the surface of CM samples was performed using cheap and simple procedure of immersing CM samples in aqueous solution of AgNO₃. The specific surface area was examined by N₂ adsorption. The pH of the aqueous slurries of the CMs samples was measured. Temperature programmed desorption method has been used in order to investigate the nature and thermal stability of surface oxygen groups before and after silver deposition. The composition and the crystallinity of silver deposits have been examined by X-ray diffraction. Chemical treatment increased a total amount of surface oxides. Consequently, the amount of deposited silver was several times higher for all chemically treated samples. The results show that the increase in the amount of CO yielding groups on CM surface leads to the enlarged Ag deposit with reduced crystallite sizes.

P.S.A.12.

SURFACE COMPLEXES FORMATION ON BORON IRRADIATED AND BORON DOPED GLASSY CARBON

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The aim of this work was to examine the influence of boron incorporation on the surface chemistry of glassy carbon. Boron incorporation was achieved in two different ways: by chemical doping (mixing phenol-formaldehyde resin with boric acid) and by B³⁺ ion irradiation of phenol-formaldehyde polymer plate before carbonization. B³⁺ ion irradiation was performed at energy of 45 keV and dose of 5x10¹⁶ ion/cm². Formation of surface oxygen groups upon subsequent exposure of the samples to the ambient air after carbonization was monitored by temperature programmed desorption. The formation of the oxygen complexes on the surface of glassy carbon was enhanced in the presence of boron. The presence of boron atoms in graphene layers in the under surface region after irradiation, alters the electron density of the whole carbon matrix. Thus, because of the ribbon structure of the glassy carbon, electronic effect of the modified under surface layer was manifested on the formation of surface oxygen groups, mainly carboxylic that desorbed CO₂ at the very low temperature, especially in the initial stage of surface oxygen groups formation. On the other hand, if boron is introduced by chemical modification, evenly distributed in the sample and present at the surface, CO₂ evolving carboxylic groups are more stable and desorbed at the higher temperature.

P.S.A.13.

CHANNEL FORMATION IN SOLID-LIQUID INTERFACE DURING DIRECTIONAL SOLIDIFICATION OF BINARY MIXTURES WITH A MUSHY LAYER

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Frequently, during directional solidification processes of binary melts or solutions the solid phase forms a rigid matrix and the liquid fills and may flow within its interstices. These regions of mixed phases are called "mushy layers". They appear ahead of the planar solidification front which becomes morphologically unstable due to the effect of constitutional supercooling. It is well-known that the brine flows developing in the solid phase (mushy layer) due to Bernoulli suction by flow of the liquid phase lead to the channel formation in the mushy layer. In this study, we present a morphological stability analysis of the mushy layer – liquid boundary which gives a new instability criterion. Our analysis is based on the heat and mass transfer equations in the mushy layer complicated by its anisotropic and inhomogeneous structure and the fluid flows in the liquid.

P.S.A.14.

INFLUENCE OF REACTIVE GRINDING PARAMETERS ON THE STRUCTURE AND PROPERTIES OF LaCaO₃ PEROVSKITE FOR PLD TARGET

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In this paper the influence of reactive grinding parameters on the structure and properties of LaCaO₃ perovskite is studied. The experiment carried out in air atmosphere for variable grinding times and different rotation speed allowed to establish optimal conditions for good quality perovskite PLD targets preparation. LaCaO₃ oxide is known as a multi-functional material. The microstructure, chemical/phase composition and morphology of obtained powders were examined by means of diverse techniques (SEM, EDS, XPS and XRD). For estimation of LaCaO₃ perovskite targets quality the nanohardness tests were performed. Obtained results confirm that high rotation speed approximately 650 RPM and elongated grinding time play the significant role for LaCaO₃ phase composition and oxide morphology.

Keywords: reactive grinding, LaCaO₃ perovskite, PLD target.

P.S.A.15.

**STRUCTURE AND PROPERTIES OF Y-DOPED Bi₂O₃ THIN FILMS
OBTAINED BY PLD TECHNIQUE**

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The paper presents the results of investigations of Y-doped Bi₂O₃ thin films obtained by PLD technique. Bismuth oxide is the material having wide application in the electronic and optical industry. The objective of our investigation is stabilization of high temperature δ phase to lower temperature, which permits take advantage of interesting properties of this material (good ion conductivity, changing conductivity with temperature) widely. The Y concentration influence on the structure and properties were studied.

The SEM, TEM, EDS and XRD investigations are presented in present paper. The adhesion to the substrate (scratch tests) and nanohardness of obtained thin films were studied. The results of investigations carried out indicate that it is possible to use produced by PLD process thin films to e.g. gas sensors, catalyst production.

Obtained results confirm that using PLD technique it is possible to carry stoichiometric composition of Y-doped Bi₂O₃ from target to single crystal substrate.

Keywords: thin films, PLD - pulsed laser deposition, yttrium doped bismuth oxide, Y-Bi₂O₃.

P.S.A.16.

**INTERMETALLICS SYNTHETIZED BY Ar⁺ ION IRRADIATION
OF NANO-LAYERED Al/Ti STRUCTURES**

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Multilayered nanometric thin films are attractive due to their properties, such as enormous hardness or unusual phase composition, which cannot be obtained in uniform bulk materials. Titanium-aluminides are promising materials for high temperature wear and corrosion protection in mechanical applications. Al/Ti multilayers were deposited in a Balzers Sputtron II system to a total thickness of 300 nm on (100) Si wafers. Ion irradiation was done with 180 keV Ar⁺ ions at normal incidence. Implanted fluences were from 1×10^{16} to 6×10^{16} ions cm⁻². The beam current was maintained at $\sim 1 \mu\text{A cm}^{-2}$, to avoid considerable beam heating of the samples. Structural and compositional characterizations were performed by Rutherford backscattering spectroscopy (RBS), X-ray diffraction analysis (XRD) and transmission electron microscopy (TEM). Nano-hardness measurements were done by Vickers method. Electrical characteristics were determined by four point probe method. Obtained results show that argon ion irradiation induces mixing between deposited Al and Ti layers. Implantation of Ar⁺ ions to fluence higher than 4×10^{16} ions cm⁻² induces the formation of AlTi₃ phase. Lateral dimensions of crystal grains in as deposited sample (~ 30 nm) rise to approximately 80 nm for implanted samples. Nano-hardness measurements show significant increase of hardness for all applied ion fluences.

P.S.A.17.

NON-CYANIDE ELECTROLYTE IN DECORATIVE AND HARD GOLD PLATING

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Gold plating is very commonly used in different areas of techniques, for decorative purposes and corrosion protection. Electrolytes based on cyanide and ferrous cyanide solutions are still present in most of gold plating baths, in spite of large efforts to replace them by some less toxic substance. Gold plating from electrolyte based on cyanide is known as high-risk technology from ecological point of view. In this work the results of synthesis a new type of electrolyte based on gold complex on mercaptotriazole based are presented. Electrolyte itself is described elsewhere. The goal was to establish the optimal parameters for decorative gold plating for this type of electrolyte and compare the results with those obtained from cyanide electrolyte. The methods used were: recording of polarization curves to obtain limiting current densities, experiments in Hull cell and experiments in laboratory cell for gold plating. All experiments were performed with additives. The same experiments were conducted with the cyanide electrolyte but with all additives normally used for decorative plating. This electrolyte can be successfully used for gold plating in comparison with expensive and risky cyanide bath. Final effect and characteristics pertaining decorative quality of gold coating are well satisfactory. Decomposition and recovery of waste solution can simply be done. Toxicity is not identified.

P.S.A.18.

KINETICS OF TITANIUM-OXO-ALKOXY CLUSTERS NUCLEATION

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The influence of titanium tetraisopropoxide $Ti(OR)_4$ ($R = ^iPr$) concentration (c - ranging from 0.04–0.07 M), molar ratio $[H_2O]/[Ti(OR)_4]$ (h - ranging from 11–20) and temperature (T - ranging from 298–318 K) was studied on the kinetics of the hydrolysis-polycondensation reaction of $Ti(OR)_4$ with H_2O in *n*-propanol solution. The isothermal kinetics of the nucleation of $Ti(OPr)_4$ was monitored by measuring absorbance changes versus time in the reaction mixture at $\lambda = 550$ nm. The isothermal rate of nucleation of titanium(IV) polyoxoalkoxides is a power law function of c and the molar concentration of water (c_w). The values of kinetic parameters α and β change complexly as h , c and T change. The value of apparent activation energy (E_a), at the investigated value of h , decreases with the increase of value c . The observed decrease in values of E_a as h increases, at $c = 0.04$ M, is an effect of the facilitated release of ROH group from the active complex at greater values of h . It was also found that nucleation is a reaction with complex kinetics whose elementary stages are hydrolysis $Ti(OR)_4$ to $Ti(OR)_3OH$ and the forming of titanium(IV) polyoxoalkoxides $[Ti_{x+y}O_y](OR)_{4x+2y}$ through the alcoxolation reaction.

P.S.A.19.

PHASE RELATIONS IN THE TITANIUM AND STANNUM COMPLEX OXIDE SYSTEM PERFORMED BY SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS

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Stannates and titanates of metals of different types have attracted much attention in recent years due to their promising application as gas sensing materials. In the present work phase formation in complex oxides systems during high-temperature self-propagating synthesis (SHS) of stannates and titanates was studied. The objects of investigation were stannates of alkaline earth metals CaSnO_3 , BaSnO_3 , transition metals FeSnO_3 , CdSnO_3 , Co_2SnO_4 , NiSnO_3 , CuSnO_3 and titanates of different compositions $\text{Cr}_{2-x}\text{Ti}_x\text{O}_3$ и $\text{Sn}_x\text{Ti}_{2-x}\text{O}_2$. SHS method is successfully used for the synthesis of such type of oxide materials. The properties of synthesized products were investigated by X-ray diffraction analysis and scanning electronic microscopy (SEM). Gas sensing tests were carried out using a microfilm technique. Propane, carbon monoxide and hydrogen were used as detecting gases. It was found that SHS of Sn-MeO systems gives less variation in phase composition than SHS of Me-SnO₂ but the main phase was the same and agreed with the required stoichiometry. After the annealing of synthesized samples at 900°C for ZnO+Sn and CoO+Sn systems the products contained the traces of SnO₂. Whilst after the annealing at 1100°C for all systems (except NiSnO₃) products were single phase. In system Ca-Sn-O the single phase product were obtained without annealing. For the most compositions of $\text{Cr}_{2-x}\text{Ti}_x\text{O}_3$ the combustion products were single phase and their gas sensing properties were investigated. It was found that compound $\text{Cr}_{1.8}\text{Ti}_{0.2}\text{O}_3$ had the best sensing properties.

P.S.A.20.

INFLUENCE OF TPA⁺ CONTENT ON SILICALITE-1 CRYSTALLIZATION

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The crystallization of silicalite-1 (MFI) was carried out on 359 K under hydrothermal condition. Precipitated silica was used as a source of silicon. Tetrapropylammonium bromide (TPABr) content, defined as TPABr/SiO₂ ratio with values in the range from 0.03 to 0.23, strongly affected rate of Silicalite-1 crystallization. Solid phase was investigated by the XRD and SEM methods. As a result of hydrothermal treatment, for investigated range of TPABr/SiO₂ ratios, silicalite-1 phase of high crystallinity was appeared.

P.S.A.21.

INFLUENCE OF Na⁺ CONTENT ON TPABr-Na₂O-SiO₂-H₂O SYSTEMS

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In the Na₂O-SiO₂-TPABr-H₂O systems, Na⁺ content was determined by Na₂O/SiO₂ ratio. This ratio was changed from 0 to 0.25. On the value equal to zero, the system was formed from SiO₂, H₂O and tetrapropylammonium bromide (TPABr), and Na⁺ was not present. Examined range of Na₂O/SiO₂ ratios is important for the crystallization of some zeolite phase, as is the silicalite-1 (MFI). Precipitated silica, structured as agglomerates of spherical nanoparticles, was used as a source of silicon. The influence of Na₂O/SiO₂ ratios on the distribution of components, between the liquid phase (mother liquor) and the solid phase, and the solid phase characteristics were investigated. The solid phase was investigated using XRD, SEM and BET methods.

P.S.A.22.

**INFLUENCE OF HYDROTHERMAL PRE-TREATMENT ON THE SYNTHESIS
OF BELITE PHASE FROM COAL FLY ASH**

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At present, belite cement synthesizing has become the hotspot in cement-concrete materials science. The favorable properties of belite in comparison with alite as well as the low CaO consuming and therefore the CO₂ emission reduction and energy saving during its fabrication have been caused the growing interest of investigation of belite cements preparing.

This paper summarizes the results of an extensive investigation of application of hydrothermal pre-treatment for synthesizing belite phase from reactive mixtures consisting of two waste kinds (bottom ash – BA and fly ash - FA) from fluidised brown coal combustion in Slovakian power plant and CaO (analytical grade reagent) addition. Starting mixtures with CaO/SiO₂ molar ratio of 2 were hydrothermally activated in rotating autoclave under various conditions. The starting mixtures and products of hydrothermal treatment were subsequently calcinated at temperatures in the range of 600 to 1200°C.

Changes in structure and phase composition of hydrothermally synthesized belite precursors and subsequent calcinated products were compared with those of starting mixtures. Based on XRD diffraction patterns and infrared spectra of pre- treatment products, the formation of the new profiles corresponding to CSH phases with low degree of ordering as belite precursors after hydrothermal treatment was confirmed. Calcination of hydrothermally treated products at 900°C led to transformation of CSH phases to wollastonite, belite and gehlenite phase. Differences in phase composition of products before and after calcination depend upon waste quality and precursor's synthesis conditions. Bottom ash isn't suitable as raw material for synthesizing belite phase because of high CaO content fixed in anhydrite form (44.1%). Coal fly ash with low CaO content in anhydrite form (4.2%) and its hydrothermal treatment in combination with subsequent heating offer opportunities for the utilization of coal fly ash as raw material for belite production.

P.S.A.23.

THE COULOMBIC CAPACITY AND CYCLE LIFE OF $\text{Li}_{1.05}\text{Cr}_{0.10}\text{Mn}_{1.85}\text{O}_4$ IN AQUEOUS LiNO_3 SOLUTION; THE EFFECT OF ADDITION OF VINYLENE CARBONATE

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The LiMn_2O_4 spinel is commonly used cathodic material for rechargeable lithium-ion batteries with organic electrolyte solvent. It is already known that the replacement of a part of Mn by other transition metal, as well as the addition of different additive to electrolyte, may help to keep the coulombic capacity (i.e. to reduce capacity fade) of this kind of material during multiple charging/discharging cycles. In order to prove the validity of these experiences in aqueous media, the Li-ion insertion in Cr-modified LiMn_2O_4 spinel with the formula $\text{Li}_{1.05}\text{Cr}_{0.10}\text{Mn}_{1.85}\text{O}_4$ was investigated by galvanostatic charging/discharging and cyclic voltammetry in aqueous LiNO_3 solution. The influence of addition of vinylene carbonate in different concentration was also studied. In an additive-free electrolyte solution, the initial capacity amounted to 80.3 mAhg^{-1} and its fade during galvanostatic charging/discharging cycles after 50 cycles amounted to even 44 %. The presence of additive in the concentration range 0.5 to 2 wt. % caused the increase of coulombic capacity and the cycle life of $\text{Li}_{1.05}\text{Cr}_{0.10}\text{Mn}_{1.85}\text{O}_4$ especially if the additive concentration was 1 wt.%. Namely, with 1wt.% of additive, the initial discharge capacity was found to amount to 112 mAhg^{-1} and, after 100th charging/discharging cycles, the capacity fade amounted to only 18%.

P.S.A.24.

SYNTHESIS AND CHARACTERISATION OF Ni(II), Co(II) AND Zn(II) PERCHLORATE COMPLEXES WITH FORMAMIDINE LIGAND

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Transition metal perchlorate complexes with nitrogen-rich formamidine ligand belong to energetic compounds. The increasing interest in new explosives is a good ground to develop safer compounds with relatively simple synthesis. In this publication the synthesis, structural and thermal properties of Ni(II), Co(II) and Zn(II) perchlorate complexes with N,N'-bis(4-acetyl-5-methylpyrazole-3-yl)formamidine (*ampf*) ligand are reported. The crystal and molecular structure of the nickel(II) complex, $[\text{Ni}(\text{ampf})(\text{H}_2\text{O})_3](\text{ClO}_4)_2$ is determined by single crystal X-ray diffraction. The complexes were characterized by IR spectrometry, powder X-ray analysis and thermal methods.

P.S.A.25.

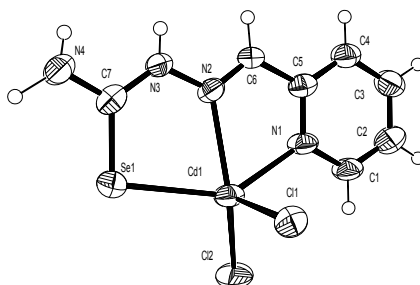
**SYNTHESIS AND X-RAY ANALYSIS OF NOVEL Cd(II) COMPLEX
WITH THE CONDENSATION PRODUCT OF 2-FORMYLPYRIDINE
AND SELENOSEMICARBAZIDE**

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In condensation reaction of 2-formylpyridine and selenosemicarbazide in presence of Cd(II) novel five-coordinated [CdCl₂(Hfpsc)]·DMSO (Hfpsc = 2-pyridinecarboxaldehyde selenosemicarbazone) complex was obtained and characterized by X-ray analysis. The molecular structure of Cd(II) complex is represented in Fig. 1, along with the labelling scheme. The neutral ligand displays a rigid planar structure and chelates the cadmium cation by a tridentate (NNSe) system involving the pyridinic and iminic nitrogen atoms and the selenium donor. This creates two five-membered chelation rings that are almost perfectly planar, while the metal is significantly displaced by 0.4 Å from the plane defined by the two chelation system. The cadmium ion completes its five-coordination by two chloride ligands, defining an irregular coordination polyhedron that is best described as a square pyramid in which the chelation (NNSe) system and one chloride ligand (Cl2) occupy the base, and the remaining chloride (Cl1) defines the apical position. The crystal packing is based on N–H···X hydrogen bonds between the NH groups of the ligand and the oxygen acceptor on the DMSO molecule, or the chloride ligand of another complex molecule.

The newly synthesized Cd(II) complex showed the cytotoxic activity similar to cisplatin.



P.S.A.26.

SYNTHESIS AND CRYSTAL STRUCTURE OF 1,2,3,4-TETRAHYDRO-9-AMINOACRIDINE TETRACHLOROZINCATE(II) MONOHYDRATE

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In the reaction of ZnCl₂ with tacrine hydrochloride in water novel tetracoordinated (C₁₃H₁₅N₂)₂[ZnCl₄]H₂O complex has been obtained and characterized by elemental analysis, molar conductivity and X-ray analysis. The structure contains two crystallographically different molecules of protonated tacrine present as counter cations, [ZnCl₄]²⁻ complex anion and one water solvent molecule. The counter cations slightly differ in puckering of the cyclohexenyl ring. The molecules of protonated tacrine are involved in different intermolecular hydrogen bonds. The π-π stacking interactions between the rings of protonated tacrine have been evidenced in the crystal. The [ZnCl₄]²⁻ complex anion has distorted tetrahedral geometry. Three out of four Cl atoms are involved in intermolecular hydrogen bonds. Intermolecular H-bond interactions that involve Cl atoms affect the Zn-Cl bond lengths.

P.S.A.27.

INFLUENCE OF SOLVENT ON THE FORMATION OF MELOXICAM-CARBOXYLIC ACID CO-CRYSTALS

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Meloxicam is a non-steroidal anti-inflammatory drug poorly soluble in water and in most of the organic solvents. One of the methods which allows to improve the bioavailability of poorly soluble drug is its co-crystallization with a suitable co-former. Seventeen co-crystals of meloxicam with different carboxylic acids were obtained by solvent-drop grinding technique using an agate mortar and SPEX 8000 vibration ball mill. In order to understand how solvent influence on the co-crystal formation, different kinds of solvents have been tested. For comparison, the co-crystals were prepared by crystallization from solution, using the same solvents. It was shown that depending on the solvent the co-crystals could be obtained in different forms or could not be obtained at all. The structures of the crystals generated by grinding and from solution were identical.

P.S.A.28.

**SYNTHESIS AND CURING OF HYPERBRANCHED RESINS MODIFIED WITH
RICINOLEIC ACID**

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The composition of alkyd resin with melamine resin is suitable for manufacturing of industrial baking enamels. In this work two hyperbranched alkyd resins based on ditrimethylolpropane as tetra functional core molecule, 2,2-bis(hydroxymethyl)propionic acid and ricinoleic acid were synthesized via an acid catalyzed polyesterification reaction. Synthesized resins were then made into enamels by mixing with commercial isobutylated melamine-formaldehyde resins, at a weight ratio 70:30. Curing of resin mixtures were investigated by differential scanning calorimetry (DSC) and Fourier transform infrared spectroscopy (FTIR). Physical, dynamic-mechanical and thermal properties of coating films were determined. It was found that the films are stable up to 300 °C and have high hardness values and good impact resistances.

P.S.A.29.

**MECHANICAL AND SWELLING PROPERTIES OF POLYURETHANE NETWORKS
WITH CONTROLLED TOPOLOGY OF NETWORK CHAINS**

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Polymer networks obtained by chemically cross-linking interpenetrating polymer chains are classical subjects of polymer physics. The cross-linking process freezes in a macroscopic connectivity between the original chains, which is related to the random conformations of the polymers at the moment of cross-linking. However, here the characteristic scale of the network structure is also determined by the averaged cross-link density and thus corresponds to the averaged size of the individual network strands, and disorder effects are restricted to rather small scales. At larger length scales the network topology can be considered as homogeneous and thus the network behaves affinely under macroscopic deformations (the simplest is given by an isotropic extension influenced by swelling). In this work we studied mechanical properties of model networks with isocyanurate rings. The temperature-insensitive damping networks are made by introducing intentionally many dangling chains in to the network. The elastomers with controlled lengths of elastically active chains are prepared in a bulk by cyclotrimerization of telechelic chains obtained from 2,4-tolyenediisocyanate, α,ω -dihydroxypoly(oxypropylene)diol, and 2-(2-methoxyethoxy)ethanol. Dynamical-mechanical properties were determined by thermal analyzer (DMTA IV, Rheometric Scientific) in the tensile mode. The evaluation of network parameters were calculated using the theory of branching processes with cascade substitution. The equilibrium swelling properties were correlated with networks structure and mechanical properties.

P.S.A.30.

**THERMAL STABILITY AND DEGRADATION OF Co(II), Cd(II) AND Zn(II)
COMPLEXES WITH *N*- BENZYLOXYCARBONYLGLYCINATO LIGAND**

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The synthesis, characterization, antimicrobial and antifungal activity of Co(II), Cd(II) and Zn(II) complexes with the *N*-Boc-gly ligand, of formulae: [Co(*N*-Boc-gly)₂(H₂O)₄]·2H₂O, [Cd(*N*-Boc-gly)₂(H₂O)₂] and [Zn(*N*-Boc-gly)₂], were described previously. The decomposition of the Co(II) and Cd(II) complexes occurs in four and decomposition of Zn(II) complex occurs in three main steps. The suggested mechanisms of thermal degradation showed that Co(II), Cd(II) and Zn(II) complexes have the same fragmentation of its ligand chains. TG curves revealed that the presence of crystallization and/or coordinated water molecules decreases thermal stability of the complexes. The observed order of decreasing stability is: [Zn(*N*-Boc-gly)₂] > [Cd(*N*-Boc-gly)₂(H₂O)₂] > [Co(*N*-Boc-gly)₂(H₂O)₄]·2H₂O, and the same trend is found after dehydration of Co(II) and Cd(II) complexes. With regard to the composition and structures of complexes it is confirmed that the loss of crystallization and/or coordinated water molecules cause a disturbance of crystal and molecular structure of the complexes resulting in thermal instability of dehydrated complexes. For determination of the apparent activation energy (E_a) and pre-exponential factor (A) Kissinger's and Ozawa's methods are used and results of these two methods are in well accordance. Friedman's method signify that the first step of degradation in the case of Cd(II) complex and the second step in the case of Co(II), Cd(II) and Zn(II) complexes are not complex in nature, whereas the first step of degradation of Co(II) and Zn(II) complexes and third step of Co(II), Cd(II) and Zn(II) complexes are the complex ones.

P.S.A.31.

THE USE OF L₉ ORTHOGONAL ARRAY WITH GREY RELATIONAL IN OPTIMIZING FRICTION WELDING PARAMETERS OF AlCuBiPb ALLOY FOR BURN OFF LENGTH AND HARDNESS

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In this study, an investigation of friction welding parameters is carried out by applying Taguchi method and grey relational analysis method. The L₉ orthogonal array (OA) is selected for this study with three parameters (rotational speed, friction pressure, forge pressure), and three levels for each parameter for optimizing multiple quality characteristics (burn off length and hardness) for joining similar aluminum alloys (AlCuBiPb type). The results for single quality (Taguchi method) optimization show that the burn off length is affected by the forge pressure, while the friction and forge pressures influence the hardness. However, the improvement of the quality of the welded joints, using the grey relational grade for multiple quality optimizations show that the optimal parameters are determined more precisely by this method. The optimal parameters obtained for this set of experiments are rotational speed 164.9 m/min, friction pressure 42 bar, and forge pressure 100 bar with 81.9 % contribution. The produced welding joints have hardness in the range of 75 to 95% of the base metal hardness for the selected set of experiments and the forge pressure is the most influencing parameter.

Keywords: Friction welding; Joining Similar aluminum alloys; Burn off length; Hardness; Taguchi and grey relational methods.

P.S.A.32.

EFFECT OF TEMPERATURE ON DODECYLMETHACRYLATE FREE RADICAL BULK POLYMERIZATION

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We have studied isothermal bulk polymerization of liquid dodecylmethacrylate by differential scanning calorimetry at temperatures 70, 80, 90 and 100 °C with 0.5 wt. % of 2, 2'-azobisisobutyronitrile as initiator. According to classic theory, it is expected that free radical polymerization starts at maximal rate and then decreases in time with consumption of monomer and initiator. However, our experimental results show that, after an induction period there is a sudden rise of polymerization rate known as autoacceleration. Polymerization rate reaches a peak and starts to decrease. Increase of temperature resulted in shorter induction period and higher peak of polymerization rate. Our results can be explained by recently published data that suggest a high organization of dodecylmethacrylate monomer.

P.S.A.33.

DETERMINATION OF HERBICIDE BROMACIL IN WATER AND SOIL SAMPLES

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A new sensitive and simple kinetic method is developed for determination of the insecticide bromacil[5-bromo-6-methyl-3-(1-methylpropyl)-2,4-(1H,3H)-pyrimidinedione]. Bromacil is one of a group compounds called substituted uracils. The method is based on reaction of oxidation sulfanilic acid by hydrogen peroxide in phosphate buffer in presence Cu(II) ion as catalyst. The insecticide bromacil shows an inhibited effect in this reaction. Bromacil was determined with linear calibration graph in the interval from 2.70 to 16.10 $\mu\text{g}/\text{cm}^3$. The developed procedure was successfully applied to the rapid determination of bromacil in soil and water samples. Solid-phase extraction (SPE) was used for extraction of bromacil from soil and water samples with Chromabond[®] (Macherey-Nagel) C18 cartridges. Solid-phase extraction (SPE) is an innovative method for efficiently and quantitatively extracting pesticides from large numbers of water and soil samples. Water sample solution was poured into a chromabond HR-P C18 cartridge and filtered through the column, and column was dried for 30 min. The sample was eluted from the column with methanol/acetone. The soil sample is shaken with a methanol/water mixture and centrifuged. The supernatant is then diluted with a concentrated NaCl solution, and drawn through an SPE column. The sorbed pesticides are finally eluted from the column with methanol. This method requires no specialized laboratory equipment and is well suited for processing large numbers of samples. Analyses of water and soil samples show recoveries of over 90%. The HPLC method was used like a comparative method to verify the results. The results obtained by two different methods showed good agreement. Reliable recovery data were found at various concentrations, after spiking water and soil, and good limits of quantification were attained.

P.S.A.34.

**XRD AND VIBRATIONAL SPECTROSKOPY INVESTIGATION
OF BaTi_{1-x}Sn_xO₃ SOLID SOLUTIONS**

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The perovskites ABX_3 represent wide group of minerals which are very important due to their excellent electrophysical properties. Unique electrical properties of perovskites are due to their crystal structure, which makes them very applicable in different area of industry. The ideal

crystal structure of the perovskites is cubic with space group symmetry $Pm\bar{3}m$. The variety of crystal structure is caused by phase transitions, which can occurs as a response to changes in temperature, pressure, and composition. The BaTiO₃ materials have the perovskite crystal structural. They have a great application in electronic industry as a dielectric and ferroelectric materials. The BaTiO₃ doped with Sn is important for practical application in ceramic capacitors as well as in functionally graded materials

In this study the crystal structure of barium titanate stagnate (BTS) BaTi_{1-x}Sn_xO₃ ($x = 0, 0.025, 0.05, 0.07, 0.10, 0.12, 0.15$) solid solutions was investigated. The structural investigations of the BTS samples were done at room temperature using an X-ray diffraction, IR and Raman spectroscopy measurements. The Rietveld refinement of the X-ray diffraction data was used to analyze the structural changes depending on amount of the Sn⁴⁺ ions in the BTS. Obtained data show that increasing of Sn amount in the structure provokes the transformation of crystal structure from tetragonal *via* mixed tetragonal/cubic to pure cubic one.

P.S.A.35.

**THE XRD ANALYSIS OF THE CALCIUM PHOSPHATES PHASE COMPOSITION
DEPENDING ON THE POWDER SYNTHESIS METHODS
AND HEATING RATES**

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The hydroxyapatite [Ca₁₀(PO₄)₆(OH)₂] (HAp) belongs to large family of calcium phosphate minerals, which have a wide application in medicine, catalysis and ecology. In the comparison with other calcium phosphate phases, hydroxyapatite possesses the highest stability at room temperature and pH between 4 and 12. However, with increasing the temperature, HAp can be partially or total transformed in the tricalcium phosphate [Ca₃(PO₄)₃] (TCP). The phase transformation of HAp into low-temperature (beta) modification of tricalcium phosphate usually starts on the temperature above 700 °C. Furthermore, the increasing of temperature above 1100 °C, leads to appearance high temperature (alpha) modification of tricalcium phosphate. Dynamics of the emergence of the particular phases as well as their relative ratio in the systems strongly depend on the heating regime, dwell time as well as the properties of the investigated powders.

In this work the influence of the different heating rates (2, 5, 10 °/min) on the HAp powders synthesized by precipitation method and hydrothermal treatment was analyzed. The dwell time at certain temperatures was 5 minutes for both systems. The evolution of the phases, their mutual ratio in the investigated systems as well as the changes of the crystallite size was estimated by the XRD analysis. Obtained data clearly indicate on significant influence of heating rate and dwell time on the phase transformation and evolution of the phases in the investigated samples.

P.S.A.36.

INFLUENCE OF ZnO NANOPARTICLES SIZE AND MORPHOLOGY ON ANTIBACTERIAL ACTIVITY AGAINST *Escherihia coli* AND *Staphylococcus aureus*

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Nanoparticle metal oxides represent a new class of important materials that are increasingly being developed for use in research and health-related applications. Although the *in vitro* antibacterial activity and efficacy of bulk zinc oxide material have been investigated, knowledge about the antibacterial activity of ZnO nanoparticles is very deficient. In this work we have synthesized ZnO nanoparticles with different size and morphologies using two kinds of procedure: hydrothermal synthesis and mechanochemical processing. Characterization of the prepared nanopowders was performed using a XRD, FE SEM, TEM technique and Malvern's Master Sizer instrument for particle size distribution.

The antibacterial behavior of ZnO nanoparticles were tested to gram-negative and grm-positive bacterial cultures, *Escherihia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*). In all examined samples, ZnO nanoparticles demonstrated a significant bacteriostatic activity.

P.S.A.37.

SYNTHESIS PROCEDURE FOR THE PREPARATION OF CaCu₃Ti₄O₁₂

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This study presents a soft green chemistry method for the synthesis of CaCu₃Ti₄O₁₂ (CCT) via an oxalate precursor. Due to its extremely high dielectric constant, this perovskite is a potential material for capacitive electronic elements. In the present study, we examined various pathways, such as coprecipitation and solvothermal reaction, to obtain a complex oxalate precursor of a proper composition for the formation of pure CCT. The phase composition and the structure of both the precursor and CCT were examined by XRPD, whereas CCT dielectric properties were measured by Wayne Kerr universal bridge B224.

P.S.A.38.

**DENSE SPHERICAL RARE OXIDE PARTICLES SYNTHESIS VIA SPRAY
PYROLYSIS OF POLYMERIC PRECURSOR SOLUTION**

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Europium-doped ($Y_{0.5}Gd_{0.5}$)₂O₃ phosphor powder is synthesized *via* spray pyrolysis of polymeric precursor solution obtained by dissolving the stoichiometric amount of corresponding metal nitrates in ethylenediaminetetraacetic acid (EDTA) - ethylene glycol (EG) mixture. The 0.1M true stable solution is obtained after pH correction with NH₄OH (final pH=8.7). Ultrasonically (1.3MHz) generated aerosol droplets are decomposed at 550 °C in argon atmosphere. Following the initial attempt for obtaining dense, nanostructured spherical particles of pure ($Y_{0.5}Gd_{0.5}$)₂O₃:Eu³⁺ phase, as-prepared dark-gray powder is additionally thermally treated for 12 h in air up to 1100 °C. The particle morphology is analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Phase identification is performed by X-ray powder diffraction (XRPD) based on which the structural refinement through Rietveld method was done. Particle chemical purity is confirmed through EDS analysis, while laser particle sizer is used for determination of the particle size distribution.

P.S.A.39.

**IMPROVEMENT OF SOLUBILITY OF DISPERSE MATERIALS
BY THE MEANS OF THE MECHANOCHEMICAL TREATMENT**

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The solubility of drug is very important factor that determines its applicability, since solubility may act as rate-limiting step in absorption and therefore may affect the bioavailability of the drug. More than 40% of potential drug products suffer from poor water solubility which frequently results in potentially important products not reaching the market or not achieving their full potential.

In this work, an effort will be invested in order to improve solubility of verapamil hydrochloride by the means of mechanochemical treatment. Influence of mechanochemical parameters and surfactants on the physicochemical properties will be examined using a XRD, FE SEM technique and Malvern's Master Sizer instrument for particle size distribution. Finally, solubility of verapamil hydrochloride will be correlated with the particle size, structural and morphological characteristics of the drug via UV-VIS Cintra 101 spectrometer.

P.S.A.40.

SOFT MECHANOCHEMICAL SYNTHESIS OF $MnFe_2O_4$ FROM THE MIXTURE OF $Mn(OH)_2$ WITH $\alpha-Fe_2O_3$ AND $Mn(OH)_2$ WITH $Fe(OH)_3$

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The influence of milling of a mixture of $Mn(OH)_2$ and $\alpha-Fe_2O_3$ and of $Mn(OH)_2$ and $Fe(OH)_3$ powders in a planetary ball mill on the reaction synthesis of nanosized $MnFe_2O_4$ ferrites was studied. The mechanochemical reaction leading to formation of the $MnFe_2O_4$ spinel phase was followed by XRD. The structure of the $MnFe_2O_4$ has been investigated by Raman spectroscopy. The obtained results are discussed and compared. We observed five active Raman modes. It can be concluded, that spinel phase formation was first observed after 3 h of milling and its formation was completed after 20 h. The synthesised $MnFe_2O_4$ ferrite had a nanocrystalline structure with a crystallite size of about 20 nm. This simple, low cost route should be applicable for the synthesis of other functional nanoparticles. The mechanochemical reaction was also followed by magnetization measurement at room temperature. Hysteresis loops are they typical of soft ferromagnetism.

P.S.A.41.

ELOUTION RATE OF MONOMERS FROM RESIN-BASED COMPOSITES CURED WITH A HALOGEN LIGHT-CURING UNIT

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Monomer conversion to polymer in resin-based composite (RBCs) is incomplete. Degree of conversion varies between 40 % and 75 %. Unreacted monomers are trapped in the polymer matrix and about 10 % may elute from RBCs. Elution of monomers from RBCs may adversely affect the biocompatibility and mechanical properties of these materials. In a clinical situation, unbounded components of RBCs may diffuse through dentine into the pulp or elute into the oral cavity. The aim of this study was to determine the elution rate of monomers UDMA and HEMA from Filtek Suprime XT after storage in 75 % ethanol/water and distilled water. Eluted monomers were quantified using high performance liquid chromatography (HPLC) after 1, 6, 24, 72, 168 and 672 hours. Based on the obtained results, elution kinetics model was proposed, based on the first order kinetics law.

P.S.A.42.

SKIN LAYERS CHARACTERISATION BY FRACTIONAL BIOIMPEDANCE

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Bioelectro-mechanical properties of skin can be very valid data for analyzing fractal characteristics of skin structure. In this paper, bioelectrical impedance method and fractional calculus have been utilized for the characterization of the human skin. Our fractional model is the generalized continuous Cole - Cole model because it predicts structural – functional parameters as a lot of Cole-Cole complex relaxation times. It is shown, using the proposed model and experimental results, that these parameters depend on the fractional indexes as a degree of the fractional derivatives in interval [0, 1]. These relaxation time constants correspond to structural – functional characteristics of the skin. The integral approximation of continual Cole – Cole model was done from ten points corresponding to orderly connected known reduced Cole-Cole elements. It was experimentally observed that five reduced Cole – Cole elements had significant values of complex relaxation times. These results open a new window of skin layer interpretation and investigation based on water well ordered nanolayers in epidermis.

P.S.A.43.

IMPROVEMENT OF CORROSION RESISTANCE AND BIOLOGICAL RESPONSES OF TITANIUM SURFACE USING ELECTROCHEMICAL ANODIZATION TREATMENT

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Titanium (Ti) has been widely used as dental implant material. The biocompatibility of Ti surface is related to the long term success of Ti dental implant. This study applied the electrochemical anodization treatment to produce a nano/submicron-scale TiO₂ mesh layer on Ti surface for dental implant application. The corrosion resistance and initial biological responses of the mesh layer were evaluated. The corrosion resistance of the test specimens was investigated using potentiodynamic polarization curve measurement in simulated oral environment. The biological responses of blood (platelet adhesion and neutrophil cell bioactivity), oral bacteria (*Streptococcus mutans* and *Streptococcus sobrinus*) and human bone marrow mesenchymal stem cells (hMSCs) on the test Ti specimens were analyzed using various biological analysis techniques. Results showed that the presence of nano/submicron-scale TiO₂ mesh layer could increase the corrosion resistance, *i.e.* decrease the corrosion current and passive current, of Ti in simulated body fluid. This mesh layer was beneficial to the initial biological responses, *i.e.* better blood coagulation and hMSCs adhesion, lower bacterial attachment, and no negative influence on neutrophil activity. We may conclude that the corrosion resistance and biological responses of Ti surface can be improved using electrochemical anodization treatment.

P.S.A.44.

MICROSTRUCTURE OF MELT SPUN Ni-Ti SHAPE MEMORY RIBBONS

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NiTi alloys are the most technologically important medical shape memory alloys (SMAs) in a wide range of applications used in orthopaedics, neurology, cardiology and interventional radiology as guide-wires, self-expandable stents, stent grafts, inferior vena cava filters and clinical instruments.

This paper discusses the application of rapid solidification by the melt spinning method for the preparation of thin NiTi ribbons for medical application. Specimens for metallographic investigation were cut from the longitudinal cross sections of melt-spun ribbons. Conventional TEM studies were carried out with an acceleration voltage of 120 kV. Additionally, the chemical composition of the samples was examined with a TEM, equipped with an EDX analyser. The phase transformation temperatures of trained ribbons were measured using a Mettler DSC 821e device (Mettler Toledo GmbH, Schwerzenbach, CH). Thermograms were recorded under static air from -40 to 180 °C at a heating/cooling rate of 10 K min⁻¹. The crystallographic structure was determined using Bragg-Brentano x-ray diffraction with Cu-K_α radiation at room temperature.

P.S.A.45.

USE OF NON-CONTACT STEREOMETRIC SYSTEM TO MEASURE MECHANICAL PROPERTIES OF BIOMATERIALS

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New optical stereometric methods are becoming commonplace in investigations of mechanical behaviour of biomaterials. An understanding of the mechanical behaviour of hard and soft tissues is of great importance in the design and investigation of biomaterials. The mechanical behaviour of biomaterials can be evaluated using a number of methods that are based on either contact or noncontact schemes for displacement measurement. The method for full field measurement of strain is done by using the ARAMIS three-dimensional image correlation system. The system uses two digital cameras that provide a synchronized stereo view of the specimen and the results show the complete strain field during the tests. Several examples are presented that highlight the use of stereometric measuring system for modern biomaterials. It is shown that this measuring methodology can capture the trends of the experiments.

P.S.A.46.

**ANALYSIS OF FATIGUE BEHAVIOUR OF TITANIUM ALLOYS
USED FOR REPLACING ARTIFICIAL JOINTS**

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Metallic biomaterials are often used in orthopedic surgery to replace structural components of the human body, such as in joint prostheses. The inside of the living body is a chemically and mechanically rough environment for biomaterials; therefore, a number of properties of the implant biomaterials are important when selecting suitable candidates for joint replacements. Biocompatibility characteristics and excellent mechanical properties of titanium alloys make them the preferred choice for such applications. This paper summarizes the fatigue, wear and corrosion resistance of titanium alloys used as biomaterials in the design of implants for artificial joints. Several examples from published sources are presented concerning total joint replacement recalls and it is shown that an understanding of the fatigue behaviour of titanium and its alloys is of prime importance in the design and investigation of artificial joint implants.

P.S.A.47.

**NON-CONTACT OPTICAL 3D DEFORMATION MEASUREMENT OF
POLYMERIZATION SHRINKAGE OF RESIN-BASED COMPOSITES USING
DIGITAL IMAGE CORRELATION**

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Dental resin-based composites (RBCs) polymerize upon light activation that triggers free radical addition of dimethacrylate monomers. As a result of this process, polymerization shrinkage of about 1-3 vol% occurs irrespective of the type of resin. The most recently developed Filtek Silorane is based on a combination of siloxanes and oxiranes in an attempt to overcome shrinkage through cationic ring opening of oxiranes. However, research has shown that even Filtek Silorane exhibits polymerization shrinkage of about 1.5 vol%. Well established methods of determination of polymerization shrinkage of RBCs include contact measurement methods, such as mercury or water dilatometry, strain gauges, the glass diaphragm and voltage transducer method. In the current study, volumetric shrinkage of several contemporary RBCs was measured using a non-contact 3D optical imaging system with two digital cameras.

P.S.A.48.

**PREPARATION OF POLYURETHANE NANOCOMPOSITE MATERIALS
BASED ON CASTOR OIL AND TITANIUM(IV)OXIDE**

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Castor oil is usually obtained by extraction from the seed of a plant (which has the botanical name *Ricinus communis*) and chemically it is an ester of fatty acids. Approximately 90% of the fatty acid content is ricinoleic acid. Due to the existence of hydroxyl groups, the oil is suitable for reactions with isocyanate compounds and polyurethane elastomeric materials preparation [1] (polymer networks [2]), adhesives and coatings. Polyurethane composites are used in a wide range of applications, such as aerospace, military, construction, electrical and electronics, medicine, transportation, marines. In recent years, polymer composites based on renewable resources have become a special interest. One of the most promising renewable materials for polymer synthesis is castor oil. Due to the existence of hydroxyl groups, the oil is suitable for polymer networks formation. The objective in this work was preparation of castor oil based polyurethanes and their composites with titanium(IV)oxide nanoparticles. Samples were formed by cast molding. For polyurethanes synthesis two types of diisocyanates, toluene diisocyanate and isophorone diisocyanate, were used without catalyst. NCO/OH ratios, r , were 1; 1,15 and 0,92. The castor oil was dried under vacuum 24h before use. FTIR spectra were recorded on tablets based on grinded polyurethanes powder and KBr. It was estimated that the properties of the samples were dependent on the NCO/OH ratio and used diisocyanate type. The polyurethane formation was confirmed by FT-IR by detection of the urethane band at 1525 cm^{-1} . It was also estimated that the OH groups from castor oil reacted with the NCO groups of the isocyanate since the broad band that corresponded to the OH groups (3430 cm^{-1}) was no longer detected or detected in reduced intensity in the urethanes spectra depending of NCO/OH ratio. The presence of the NCO free groups was detected only for sample with $r=1,11$ (band at 2300 cm^{-1}). For nanocomposite preparation titanium(IV)oxide filler loadings were in the range from 0,5 to 2 wt%. Glass transition temperatures (determined from DSC measurements) were in range -13 to 0°C . Tg values decrease with increasing filler content.

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P.S.A.49.

**SELF ASSEMBLING OF BIOMIMETIC HYDROXYAPATITE
ON THE SURFACE OF DIFFERENT POLYMER THIN FILMS**

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Self assembling of biomimetic calcium hydroxyapatite on the surface of polymer thin films was investigated in this paper. Polymer films (alginate, cellulose and PLGA) were previously deposited on the surface of porous hydroxyapatite thin film. These films were kept in slightly modified simulated body fluid (SBF) for six weeks, on the temperature of 37°C. After aging in SBF, samples were investigated by FTIR-ATR to analyze obtained phases, while morphology of self assembled hydroxyapatite was investigated by SEM.

P.S.A.50.

**THE EFFECT OF STRUCTURAL CHANGES ON FUNCTIONAL PROPERTIES
OF METASTABLE ALLOY $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_3\text{Si}_{15.5}\text{B}_7$**

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This paper investigates the effect of structural changes of ribbon-shaped amorphous alloy $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_3\text{Si}_{15.5}\text{B}_7$ during the annealing process on its functional properties. DSC method was used to determine temperature range of thermal stability of $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_3\text{Si}_{15.5}\text{B}_7$ alloy. It has been shown that this alloy is stable up to 500°C. The effect of structural relaxation process on magnetic properties of this alloy has been investigated through thermomagnetic measurements by Faraday method, in the temperature range from room temperature up to 450°C. The same temperature range was used to investigate the effect of structural relaxation process on the electron density change at Fermi level, upon a number of annealings, by measuring the thermoelectromotive force. Upon a number of successive annealings of the same sample along with gradually higher annealing temperature, it has been shown that magnetic susceptibility of this alloy may be increased by up to 40%. The measurements reflecting resistivity changes in isothermal conditions at temperatures of $t_1 = 420^\circ\text{C}$, $t_2 = 435^\circ\text{C}$ and $t_3 = 450^\circ\text{C}$ during the time interval of $\tau = 20$ minutes have determined kinetic parameters and activation energies of relaxation processes. It has been shown that the structural relaxation process occurs in two stages. The first stage is kinetic process, whereas the second is diffusion process. Activation energy of the first stage equals $E_1 = 139,43$ J/mol K, and of the second $E_2 = 184,07$ J/mol K.

P.S.A.51.

**KINETICS OF STRUCTURAL RELAXATION
OF NANOSTRUCTURAL POWDERS Ni AND Co**

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Nanostructural powders Ni and Co were obtained from ammonium solution by electrochemical deposition at the current density of 400mA/cm², at room temperature. The structure and morphology of the obtained powders were investigated by SEM microscopy method. It was shown that Ni powder contains 36,14% Oxygen, whereas Co powder contains 17,13% Oxygen. The effect of structural relaxation and crystallization on magnetic properties was tested by thermomagnetic measuring, in temperature interval from room temperature to 550°C, during multilevel successive heatings of the same sample. It was shown that the structural relaxation caused the increase of magnetic permeability of nanostructural Co powder and Ni powder by 14%, and 22% respectively. After the crystallization process, magnetic permeability of Co powder decreased for 10% in relation to starting powder, whereas magnetic permeability of Ni powder decreased by about 7% in relation to relaxed powder. The process of structural relaxation of these powders was tested by thermomagnetic measuring under isothermal conditions at T₁=160°C, T₂=180°C, T₃=200°C, for Co powder, and T'₁=180°C, T'₂=200°C, T'₃=220°C, for Ni powder. It was shown that the process of structural relaxation of both powders was performed at two levels. The first level of the structural relaxation of both powders was kinetic process and the other was slow diffusion process. Constant velocity and the process activation energy were estimated for both levels of the structural relaxation process.

Keywords: Co, Ni nanostructural powders, kinetics, structural relaxation.

P.S.A.52.

THE EFFECT OF CHANGE IN ELECTRON STATE DENSITY AT FERMI LEVEL DURING THE MECHANICAL STRAIN ON SENSITIVITY COEFFICIENT OF THE RIBBON-SHAPED AMORPHOUS ALLOY $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$ AS FORCE SENSOR

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Amorphous alloy $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$, annealed at 400°C for 30 minutes, can be used as force sensor in temperature range from 0°C to 300°C. The alloy has stable structure in this temperature range, marks low temperature resistivity coefficient and linear dependence of resistivity upon strain intensity. Crystallization process in annealed ribbon occurs only in the temperature range from 500°C to 560°C.

This paper has identified and determined the correlation between the strain intensity of the amorphous alloy $\text{Fe}_{81}\text{B}_{13}\text{Si}_4\text{C}_2$ and its sensitivity coefficient k . On the basis of experimentally obtained dependance rates of termoelectromotive force (TEMF) upon temperature and strain intensity, it has been proved that electron state density at Fermi level decreases with greater strain. This causes an increase in resistivity of the ribbon-shaped alloy, and consequently results in its larger sensitivity coefficient. Strain of 200 MPa of the ribbon leads to a relative change in density of electron state at Fermi level of approximately 5,21%, as compared to the ribbon strained at 50 MPa. Relative change in electron state density corresponds to the relative change in sensitivity coefficient of 58,4%.

P.S.A.53.

CORRELATION BETWEEN HYDROGEN PRESSURE CHANGE AND RESISTIVITY CHANGE DURING HYDROGEN ABSORPTION ON NON PALLADIUM-COATED AND PALLADIUM-COATED COBALT POWDER

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DSC method was used to investigate the process of hydrogen absorption on palladium-coated cobalt powder (0,003% Pd). Furthermore, hydrogen absorption process was also investigated via measurement of absorbent resistivity and corresponding change in hydrogen pressure during absorption. It has been shown that hydrogen absorption causes increase in resistivity of cobalt powder and subsequent fall in hydrogen pressure in the chamber.

The investigation proved that hydration enthalpy of non palladium-coated cobalt powder equals 85,9 J/g, while in case of 0,02% Pd coated cobalt powder, it amounts to 3,46 J/g. The process of hydrogen absorption on non palladium-coated powder occurs in temperature range from 140⁰C to 280⁰C, whereas for palladium-coated powder it requires the temperature range from 80⁰C to 240⁰C. The measurement of hydrogen pressure during hydration has shown that the number of absorbed hydrogen atoms on palladium-coated powder is, depending on the temperature, 4,9 times bigger than on non palladium-coated powder, at the temperature of 160⁰C for the same amount of time.

P.S.A.54.

MICROSTRUCTURAL AND MAGNETIC PROPERTIES OF ELECTROCHEMICALLY DEPOSITED Ni_xFe_yW_z ALLOY

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A nanostructured nickle-iron-tungsten alloy powder was obtained by electrochemical deposition from ammoniacal citrate bath. The chemical composition, microstructure and morphology of the powder are dependent upon bath composition and deposition current density. Current efficiency decreases and the alloy content of iron and tungsten increases with increasing deposition current density. X-ray analysis (XRD) shows formation of the FCC phase in the alloy. An increase in deposition current density results in a decrease in crystal grain size. The amorphous Ni_xFe_yW_z powder is produced at high current densities $j > 300 \text{ mAcm}^{-2}$. Differential scanning calorimetry was used to assess the thermal stability of the powder. Annealing the nanostructured Ni_xFe_yW_z powder at low and high temperatures promotes structural relaxation and crystallisation, respectively. The temperature range for the processes shifts to higher temperatures as the alloy content of tungsten increases. The magnetic permeability of the alloy decreases with increasing tungsten content of the alloy. Annealing the alloy at temperatures somewhat lower than the crystallisation temperature range leads to a 30 percent increase in magnetic permeability.

Key words: nanostructured nickle-iron-tungsten alloy powder, magnetic permeability.

P.S.A.55.

**MAGNETIC PROPERTIES OF FeCoV ALLOY
PREPARED BY POWDER INJECTION MOLDING**

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In this study, Fe₄₉Co₄₉V₂ magnets produced by powder injection molding (PIM) technology have been investigated. The feedstock for PIM was prepared by mixing starting FeCoV powder with a low viscosity binder. Green samples of torroidal shape were subjected to solvent debinding and subsequent thermal debinding followed by sintering. Sintering was performed during 3.5 hours: from 1370 °C to 1460 °C in hydrogen atmosphere or from 1330 °C to 1400 °C in vacuum.

Magnetic measurements were performed by Faraday balance and by B-H hysteresis graph at frequency of 50 Hz. Temperature dependence of the magnetic susceptibility of sintered samples was investigated by the modified Faraday method in the temperature region from room temperature up to 550 °C. It has been established that the Curie temperature is about 250 °C.

Sample sintered in vacuum at 1330 °C has the lowest coercivity $H_C \approx 1450$ A/m and saturation $B_s \approx 1.04$ T. Sample sintered in hydrogen at 1370 °C has the coercivity $H_C \approx 2100$ A/m and improved saturation of $B_s \approx 1.4$ T. Hysteresis loops obtained by increasing excitation up to $H_m = 8$ kA/m were used for estimation of dependence of relative permeability μ_r vs. magnetic field H . For the sample sintered in vacuum at 1330 °C it can be observed the maximum of about $\mu_r \approx 400$ at excitation of 1 kA/m followed by constant decrease up to $\mu_r \approx 100$ at excitation of 8 kA/m. For the sample sintered in hydrogen at 1370 °C it can be observed the maximum of about $\mu_r \approx 270$ at excitation of 2 kA/m followed by constant decrease up to $\mu_r \approx 150$ at excitation of 8 kA/m.

P.S.A.56.

CHARACTERISTICS OF ELECTROCHEMICALLY DEPOSITED Ni_xCo_y ALLOY POWDER

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A nanostructured Ni_xCo_y alloy powder was obtained by electrochemical deposition from ammoniacal bath. X-ray analysis shows that the alloy is a mixture of crystals of solid solutions of nickel and cobalt having the face-centred cubic (FCC) and hexagonal close-packed (HCP) structures. As deposition current density increases, current efficiency and deposited crystal grain size decrease, and the alloy content of nickel and FCC phase increases. Amorphous phase is obtained at higher current densities. Its proportion in the alloy increases with an increase in both nickel content of the solution and deposition current density. Annealing the powders at temperatures higher than 750°C leads to the crystallisation of the amorphous structure into the FCC phase, HCP-FCC phase transition, growth of crystal grains of the FCC phase, and a decrease in both the minimum density of chaotically distributed dislocations and the average microstrain value. Both shape and size of the electrochemically obtained powder are dependent upon the nickel content of the solution and deposition current density. The powder having a high nickel content is cauliflower-shaped. An increase in the alloy content of cobalt induces the deposit morphology to change from the cauliflower-like structure to a parquet-like structure. The deposits produced at high current densities are observed to be covered with needle-like crystalline dendrites and craters where hydrogen is evolved. Differential scanning calorimetry (DSC) shows that the thermal stability of the alloys increases with increasing nickel content. Structural relaxation and crystallisation occur at temperatures higher than 200°C and 390°C, respectively. The above structural changes induce a decrease in the electrical resistivity of the Ni_xCo_y alloy. Annealing the Ni_xCo_y alloys within the structural relaxation temperature range results in a decrease in electrical resistivity and an increase in magnetic permeability.

Key words: nanostructured alloy powder, electrical resistivity, magnetic permeability

P.S.A.57.

**A NOVEL CATALYST FOR THE ELECTROCHEMICAL REDUCTION
OF D-XYLOSE TO XYLITOLE**

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A zinc-nickel-tin alloy coating was electrodeposited from a sulfate bath onto a copper mesh. The coating was immersed for some time in 0.1 mol dm⁻³ HgCl₂ solution to obtain its amalgam. The amalgamated nanostructured coating has good mechanical properties and can be used as a suitable catalyst for the reduction of xylose to xylitol. During the electrochemical production of xylitol by electrolysis of an aqueous solution containing xylose and Na₂SO₄ as the basic electrolyte, two parallel reactions take place on the cathode: the desired reduction of the oxycarbonyl form of D-xylose obtained by mutarotation to xylitol and the undesired hydrogen evolution reaction. The microstructure of the nanocrystalline amalgam favours the reaction between H_{ad} and the oxycarbonyl form of D-xylose, thus providing a high current efficiency for xylitol production at current densities up to 150 mA cm⁻². Current efficiency increases with increasing xylose concentration and decreasing current density. Maximum xylitol yield is obtained at a pH range of 6.0 < pH < 8.5 as the lowest rate of D-xylose to 1-deoxy pentose reduction, D-xylose to lyxose isomerisation and lyxose to deoxy pentose reduction occurs within the said pH range.

Key words: electrochemical reduction, D-xylose, xylitol, nanostructured catalyst

P.S.B.1.

STRUCTURAL AND MAGNETIC PROPERTIES OF $Y_{1-x}Gd_xTiO_3$ SOLID SOLUTION

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In this work we investigated structural and magnetic properties of novel polycrystalline samples $Y_{1-x}Gd_xTiO_3$ ($x = 0, 0.25, 0.5, 0.75$ and 1). All the samples were prepared by the arc-melting of appropriate mixture of Y_2O_3 , Gd_2O_3 , TiO_2 and Ti in argon atmosphere. X-ray diffraction revealed that the crystal structure of $Y_{1-x}Gd_xTiO_3$ solid solution is a pseudocubic perovskite with an orthorhombic distortion (the $GdFeO_3$ -type distortion). The magnetic properties of these materials are concentration and temperature dependent. The $Y_{1-x}Gd_xTiO_3$ system has been shown to exhibit a long-range magnetic-ordering temperature that increases systematically with the increase of the Gd concentration (from 29 K for $YTiO_3$ to 35 K for $GdTiO_3$). The saturation magnetization also increases with the increase of the Gd concentration.

P.S.B.2.

$LYO_3:Sm^{3+}$ AND $LYO_3:Tb^{3+}$ NANOPHOSPHORS: PREPARATION AND PHOSPHORESCENCE PROPERTIES

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Samarium and terbium doped $LaYO_3$ nanocrystalline phosphor powders are obtained by polymer complex solution method. Stoichiometric quantities of La_2O_3 , Y_2O_3 and for dopant ions Sm_2O_3 or Tb_4O_7 were dissolved in hot nitric acid. Polyethylene glycol was added in solutions in 1:1 mass ratio to corresponding metal nitrates to form gel. The gel is combusted and annealed at 800 °C for two hours to form nanopowder samples. Crystalline structure and phase purity is checked by X-ray diffraction. Luminescence properties of Sm^{3+} and Tb^{3+} doped Lu_2O_3 exhibited characteristic red emission (coming from the intra-4f-shell $^4G_{5/2} \rightarrow ^6H_J$ electron transitions) and pseudo-white emission (coming from intra-4f-shell $^5D_4 \rightarrow ^7F_J$ electron transitions), respectively. Emission spectra and emission kinetics dependence on temperature are investigated in the range from 10 K to room temperature.

P.S.B.3.

**JUDD-OFELT ANALYSIS OF EMISSION FROM $Y_2O_3:Eu^{3+}$
TRANSLUCENT CERAMICS**

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Europium doped yttrium oxide nanocrystalline powders were prepared using polymer complex solution method utilizing polyethylene glycol (PEG) of different molecular weights. Then, the powders were cold-pressed under the pressure of 800 MPa and subsequently sintered at 1200°C for 18h to form translucent phosphorescent ceramics. X-ray diffraction measurements confirmed that pure Y_2O_3 phase has been obtained for all samples, while scanning electron microscopy observations showed that powder morphologies differs with different molecular weights of used PEGs. Optical properties were examined by photoluminescence spectroscopy and spectra of all samples showed intense red emission, typical for f-f electronic transitions of the Eu^{3+} ions. Judd–Ofelt theory was applied to analyze experimental data for the quantitative determination of ceramics optical parameters such as $\Omega_{2,4}$ Judd–Ofelt parameters, radiative and nonradiative transition rates and emission quantum efficiency.

P.S.B.4.

**RAMAN SPECTROSCOPY STUDY OF $Bi_{12}SiO_{20}$ AND $Bi_{12}GeO_{20}$
SINGLE CRYSTALS PREPARED BY THE CZOCHRALSKI TECHNIQUE**

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Single crystals of bismuth silicon oxide ($Bi_{12}SiO_{20}$) and bismuth germanium oxide ($Bi_{12}GeO_{20}$) are promising materials for various applications. These crystals exhibit photoconducting, photoluminescent and piezoelectric properties. They single crystals were grown by the Czochralski technique. The critical diameter and the critical rate of rotation were calculated. Suitable polishing and etching solutions were determined. The structure of the $Bi_{12}SiO_{20}$ and $Bi_{12}GeO_{20}$ has been investigated by X-ray diffraction and Raman spectroscopy. The obtained results are discussed and compared. We observed 20 active Raman modes. It can be concluded, that the three new modes are not found in the published literature.

P.S.B.5.

PHOTOCATALYTIC HYDROGEN PRODUCTION BY SEMICONDUCTOR HETEROJUNCTION MATERIALS

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The photocatalytic decomposition of water with a semiconductor under visible light attracts increasing interest because the attempt is aimed not only at producing hydrogen from water utilizing solar energy, but also at finding methods of making use of the photosynthetic process as green plants for direct production.

In this talk, we will introduce advance and development of photocatalysis and hydrogen energy research in our group for the relative research project. It was observed that the photocurrent and the incident photon to current conversion efficiencies (IPCE or external quantum efficiencies) of these heterojunction were higher than that of the singles, particularly under visible light irradiation. These semiconductor heterojunction electrodes have potential to be a photoanode for hydrogen production under sunlight illumination.

We found some new series of oxide semiconductor photocatalysts. These photocatalysts have different crystal structure, leading to different electronic structures. Their photocatalytic degradation of organic contaminants was investigated systematically, by selecting acetaldehyde as a model gaseous contaminant, chloroform as a model solvent contaminant and methylene blue (MB) as a model dye contaminant, respectively.

P.S.B.6.

CALCULATIONS OF MOLECULAR STRUCTURES AND PROCESSES IMPORTANT FOR HYDROGEN BEHAVIOUR IN THE Li-AMIDE/IMIDE SYSTEM

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Lithium amide (LiNH_2) and imide (Li_2NH) have recently attracted much attention as part of the Li-H-N system possibly suitable for hydrogen (H) storage applications. However, the ground state imide structure is still unknown with at least six candidate structures, exhibiting energy values all very close to one another. In order to discover possible pathways of the imide-amide-imide transformations during the hydrogen absorption/desorption cycles, we have examined the molecular structures involved (along with their changes during these processes) using *ab-initio* calculations based on the linear combination of atomic orbitals (LCAO). In addition, the influence of Li substitution with some other elements of interest, and the influence of this replacement on the system behaviour were investigated. These analyses were complemented by density functional theory (DFT) calculations of several crystal structures appearing in the processes. In that way a thorough insight into the structures and the processes taking place at atomic level is attained, providing a starting point for understanding of these complicated systems of a great practical importance, and the mechanisms governing their transformations.

P.S.B.7.

5 NM STRUCTURES PRODUCED BY DIRECT LASER WRITING

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3D modifications of optical properties of transparent materials using laser irradiation are interesting in both the scientific and technological aspects. There is a resolution barrier due to the optical diffraction. Here we present a new approach to overcome diffraction limit by using novel materials. In this paper, we report experimental results obtained by HRTEM and optical absorption spectroscopy, for a fluorescent photosensitive glass-ceramics containing rare earths ions such as samarium (Sm). Using a home built dynamic tester, with a low power laser, we recorded nanostructures having 5 nm line width. In the line structure, measurements reveal the presence of silver nanocrystals with few nanometer size. HRTEM shows that there is a random orientation of the nanocrystals. A writing mechanism with three steps was proposed.

P.S.B.8.

SYNTHESIS AND CHARACTERIZATION OF PURE AND DOPED Ba(Mg_{1/3}Ta_{2/3})O₃ NANOPOWDERS

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Preparation of Ba(Mg_{1/3}Ta_{2/3})O₃ ceramic materials (BMT) with optimal properties for specific applications requires special synthesis parameters and thermal treatments due to the difficult control of stoichiometry and cation ordering. In order to improve sinterability conditions and microwave dielectric properties, different dopants as oxides were introduced in perovskite structure formed at low temperatures. The Pechini modified method for compound syntheses were established. XRD, DTA, FTIR, TEM, SEM and EDX were employed for compositional, structural and morphological characterizations of nanopowders. BMT nanopowders synthesized by Pechini method show 13 nm medium diameter of grain size and promote hexagonal structure. Correlations between nanopowder characteristics and dopant quantities, synthesis methods and thermal treatments were established. The dielectric properties were measured in the microwave range for different BMT samples.

P.S.B.9.

**ROOM-TEMPERATURE FERROMAGNETISM IN Zn-Mn-O,
X-RAY PHOTOEMISSION SURFACE STUDY**

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The existence of ferromagnetism in Zn-Mn-O semiconductor samples and dependence on the preparation condition were systematically investigated. Samples with manganese concentration ranging from 0 to 10 at%, were prepared by a solid state reaction route using metal-oxalate precursors. Thermal treatment was carried out in air at temperatures ranging from 400 to 900°C. The samples were investigated by X-ray diffraction, transmission electron microscopy, magnetization measurements and XPS spectroscopy. XPS analyses of surface composition, chemical bonding and XPS depth profiling were successfully employed on powder revealing the chemical composition at the surface of the grains and underneath. The present investigation emphasizes important role of the grain surface in observed room temperature ferromagnetism. It seems that the ferromagnetic phase is correlated with oxygen build up at the surface.

P.S.B.10.

**MAGNETIC PROPERTIES OF Mn-OXIDE NANOPARTICLES
DISPERSED IN AN AMORPHOUS SiO₂ MATRIX**

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Samples of Mn-oxide nanoparticles dispersed in an amorphous SiO₂ matrix with manganese concentration 0.7 and 3 at % have been synthesized by a sol-gel method. Transmission electron microscopy analysis has shown that the samples contain agglomerates of amorphous silica particles 10 – 20 nm in size, and two types of Mn-rich particles, smaller Mn-rich nanoparticles with dimensions between 3 and 10 nm, and larger crystalline areas consisting of aggregates of the smaller nanoparticles. High-temperature magnetic susceptibility study reveals that dominant magnetic phase at higher temperatures is λ -MnO₂. At temperatures below $T_c = 43$ K strong ferrimagnetism originating from the minor Mn₃O₄ phase masks the relatively weak magnetism of λ -MnO₂ with antiferromagnetic interactions. Magnetic field dependence of the maximum in the zero-field-cooled magnetization for both the samples in the vicinity of 40 K, and a frequency shift of the real component of the ac magnetic susceptibility in the sample with 3 at % Mn suggest that the magnetic moments of the smaller Mn₃O₄ nanoparticles with dimensions below 10 nm are exposed to thermally activated blocking process just below the Curie temperature T_c . Appearance of a maximum in the zero-field-cooled magnetization for both the samples below 10 K indicates possible spin glass freezing of the magnetic moments at low temperatures which might occur in the geometrically frustrated Mn sublattice of the λ -MnO₂ crystal structure.

P.S.B.11.

**SEGMENTED THERMISTORS PRINTED USING NTC NANOMETRIC PASTE
ON ALUMINA AND Sr-FERRITE SUBSTRATES**

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Thick film planar segmented NTC thermistors based on nanometer powder of complex spinel (NiMn₂O₄ doped with CuO) were screen printed on alumina and Sr-ferrite substrates. New planar thermistor geometry was applied to prepare custom designed temperature and water flow sensors. The influence of type of substrates and thermistor geometry on sensor characteristics were described. Particular attention was paid to their electronic and thermal properties with intention of forming a sensor with the most suitable thick film geometry and optimal electrical and time response.

P.S.B.12.

**THE INFLUENCE OF THE ATMOSPHERE AND IMPULSE EFFECT OF EXTERNAL
MAGNETIC FIELD ON THE MAGNETIC FEATURES OF MnZn-FERRITE
DURING THE PROCESS OF SINTERING**

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The sintering of the pressed MnZn-ferrite powder samples was performed at the temperature of 1340°C, during 3.5h, in the atmosphere of air, argon, nitrogen, and in the vacuum.

Two types of samples were sintered:

1. the samples that were subjected to the effect of external magnetic field of $11 \cdot 10^3 \text{ A/m}$ at every 20°C during the heatings to 600°C
2. starting samples that were only pressed

It was shown that magnetization of the samples which had previously been subjected to the effect of external magnetic field, increased by about 10% in relation to the starting samples after the sintering at 1340°C. At the same time, magnetization of both types of samples sintered in the atmosphere of air was about 20% higher than magnetization of the samples sintered in the atmosphere of argon, nitrogen and in the vacuum. Measuring of specific electrical resistance of all the samples showed that the samples sintered in the air had specific electrical resistance of ceramics, whereas the other samples had specific electrical resistance of metal. It was shown that the samples sintered in the air atmosphere had properties of hard ferromagnetic elements, while the other samples had properties of soft ferromagnetic elements. All the magnetic and ferromagnetic measurements were performed according to Faraday's method, whereas the measurements of specific electrical resistance were performed according to the Four-point method.

P.S.B.13.

THE INFLUENCE OF THE PORE GEOMETRY ON THE MECHANICAL PROPERTIES OF POROUS HAP-BASED BIOCERAMICS

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In this study, the influence of the shape, size and volume fraction of the pores on the mechanical properties of the porous HAP-based bioceramics was investigated. A three-dimensional, finite element unit cell model was applied to evaluate the influence of pore shape and volume fraction on the mechanical strength and stiffness of HAP ceramics. Obtained results suggests that porous HAP with sphere-like pore shapes generates lower values of the stress concentration factor and therefore better strength properties compared to crack-like pore shapes. The region of the pores where the maximum stress occurs is in certain conditions the favorable place for local flaw deformation as well as crack initiation and propagation. From this point of view porous material with sphere-like pores has more resistance to fracture than material with crack-like pore shapes. Conducted experimental analysis confirmed that porous HAP with sphere-like pores have better mechanical properties compared to non-spherical pore shapes.

Keywords: bioceramics, porosity, hydroxyapatite, mechanical properties, finite element modeling.

P.S.B.14.

HIGH TEMPERATURE OPTICAL SPECTROSCOPY OF REDUCED AND N-DOPED TiO₂

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Titanium dioxide, TiO₂, is one of the most promising photocatalyst for applications in environmental protection and renewable energies. Its photocatalytic efficiency can be enhanced by tailoring the defect structure of TiO₂ lattice via reduction or doping. The optical absorption of N-doped TiO₂ has been found to extend from UV to the visible range. With the aim to understand the mechanism of oxygen substitution by nitrogen in oxides, we have studied the oxidation behavior of reduced TiO₂ and of N-doped TiO_{2-x} in the form of thin films and in the form of powders by means of in-situ optical spectroscopy at elevated temperatures. The oxidation kinetics will be discussed in terms of a microscopic model involving lattice defects and their diffusion.

P.S.B.15.

LOW TEMPERATURE MAGNETIC PROPERTIES OF $\text{Pr}_{0.7}(\text{Ca,Sr})_{0.3}\text{CoO}_3$ OXIDES

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The transition metal oxides display remarkable magnetic and transport properties of interest for technical applications. Doped cobaltite perovskites $\text{Ln}_{1-x}\text{A}_x\text{CoO}_3$ ($\text{Ln} = \text{La}$, rare earth and $A = \text{Ca}$, Sr , Ba), have recently attracted much attention due to their unique feature to change the spin-state of the Co^{3+} and Co^{4+} ions from low- to intermediate- or high-spin state. In the present work, the physical properties of the $\text{Pr}_{0.7}(\text{Ca}_{1-x}\text{Sr}_x)_{0.3}\text{CoO}_3$ cobaltites have been investigated when the average size of the interpolated cation was changed. These changes strongly influence the structure and consequently the magnetotransport properties. Structures were characterized by X-ray diffraction. The magnetic measurements were done over a wide temperature and magnetic field ranges. $\text{Pr}_{0.3}\text{Ca}_{0.7}\text{CoO}_3$ has an orthorhombic $Pbnm$ symmetry and it shows a semiconducting type behavior over the whole temperature range. Below 70 K this sample has and a magnetic cluster-glass behavior as suggested from frequency dependent ac susceptibility measurements. $\text{Pr}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$ has a monoclinic ($P2_1/m$) structure and it has a metallic type behavior. Our ac susceptibility data showed a frequency dependent peak in $\chi'(T)$ at $T_C \approx 230$ K and a broad maximum at $T_A \approx 110$ K. This magnetic behavior was also confirmed from muSR measurements. With increasing Sr concentration x , the magnetic cluster-glass phase turns, gradually, to a ferromagnetic one. The low temperature phase transition at T_A can be seen only above $x \approx 0.95$. All the ferromagnetic samples showed high magnetocaloric effect. The electrical and magnetic properties of these compounds can be tuned by the Ca/Sr concentration ratio. The possible physical origin of these phenomena is discussed in the context of structural changes in the presence of magnetic clusters and spin transitions due to the multiple spin configurations of the cobaltites.

P.S.B.16.

**STRUCTURAL CHARACTERIZATION OF SILICA MICRO LAYERS
THERMALLY GROWN ON SiC AND Si-C-N BULK CERAMICS**

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The structure of thermally grown protective silica layers can be composed of amorphous and/or polycrystalline silica phases, each having different structural imperfections that provide a fast path for oxygen transport. For a better understanding of the oxygen diffusion mechanism along the high-diffusivity paths, detailed structural characterization of silica layers has to be employed. In this work, the structure of silica layers grown on Si-C-N and SiC substrates at 1673 K in ambient air for 48 h will be studied by use of X-ray Diffraction (XRD), Micro-Raman Spectroscopy, Scanning Electron Microscopy with Energy Dispersive System (SEM-EDS) and Transmission Electron Microscopy equipped with an Electron Diffraction Analyzer (TEM/ED). Results will be correlated with the recently proposed short-circuit oxygen diffusion mechanism.

P.S.B.17.

IMPROVEMENT OF HYDROGEN STORAGE PROPERTIES OF MgH₂ BY α AND β SiC

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Besides high volumetric and gravimetric density and low cost, the high thermodynamic stability and high desorption temperature are severe problems for the application of MgH₂ as H storage material. Hence, the research activities are focused on modification of MgH₂ by structural destabilization such as: addition of impurities and/or catalysts by ball milling or ion bombardment. The ball milling of powder samples leads to its crystallite and particle size refinement, surface modification and metastable phase formation, which generally promote the reaction of MgH₂ decomposition. It has been reported that SiC mechanically milled either with pure Mg in H atmosphere or with MgH₂ leads to formation of SiC/MgH₂ composite with reduced grain size and increased surface area of MgH₂, which is beneficial to the H sorption properties. It was also demonstrated that it is necessary to limit the amount of SiC since its large quantity block the H diffusion path due to formation of large agglomerates. In our work we investigated the H storage properties of composites obtained by ball milling of MgH₂ with two different crystallographic SiC phases (α and β) to emphasis the effect of crystallographic variation to the morphology of samples and consequently on desorption properties. MgH₂/SiC composites were prepared by ball milling in Turbula Type 2TC Mixer of commercial MgH₂ powder with 5 wt% α -SiC (mean particle size 1.2 μ m) and β -SiC (mean particle size 1.4 μ m) under Ar atmosphere and BPR=10:1 for 10 h. XRD analysis was done by means of Siemens KRISTALLOFLEX D-500 device. Malvern 2000SM Mastersizer laser scattering particle size analysis system was used to obtain the quantitative MgH₂ particle size distributions. A VEGA TS 5130MM, Tescan Brno SEM equipped with EDS detector was used to obtain the phase distribution, the material homogeneity and the morphology of the powder grains. The H desorption properties were investigated by DSC analysis using DSC 151R Setaram Instruments. Sample milled with hexagonal SiC show the agglomerates of about 70 μ m while in the sample milled with cubic SiC there are no such agglomerates. Much better additive distribution in MgH₂ matrix in sample milled with 5wt % of cubic SiC can be also seen. The particle size distribution is bimodal in both cases: ~ 30% of particles with diameter smaller than 1 μ m and ~ 70% of particles has main diameter smaller than 10 μ m. Such microstructure promote desorption properties of composites since both milled samples show lower desorption T of 45 °C than unmilled MgH₂, while the earlier T onset (about 200°C) shows only cubic SiC.

P.S.B.18.

**INTERACTION OF A HYDROGEN ATOM WITH GRAPHITE (0001) SURFACE
– A SEMIEMPIRICAL APPROACH**

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We have theoretically investigated hydrogen chemisorption on graphene by applying semi-empirical quantum chemical method. Three dynamic routes of an H-atom approaching the graphene surface have been compared in relation to the H-atom sticking. It has been found that the approach along the ortho/para direction, under the angle of incidence of 60° , increases sticking probability compared to the collinear case, when H-atom approaches perpendicularly to the graphene surface. Also, the results of the dynamic calculations have shown that the first nearest neighbors of the targeted carbon atom play crucial role in hydrogen chemisorption. It has been observed that the formation of molecular hydrogen over Eley-Rideal mechanism with steering occurs at the very narrow region of the kinetic energy of the impinging H-atom. The binding energies, and vibrational and structural parameters determined from static and dynamic calculations by using the semiempirical approach were in excellent agreement with those calculated by employing a more sophisticated methodology.

P.S.B.19.

**PLASMON – IONISED IMPURITY – INTERACTION
IN Co AND Ni DOPED PbTe**

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Far – infrared reflection spectra in wide temperature range were used to investigate the vibrational properties of the PbTe single crystals doped with Co and Ni. In the analysis of the experimental results we used dielectric function that took into account the existence of plasmon – ionised impurity – phonon interaction. The results obtained from the experimental spectra as the best fit, are in very good agreement with the theoretical prediction. Together with the strong coupling we obtained three local modes of Co and Ni, which corresponded to the impurity atoms in different valence states. The positions of these modes depend on the impurity center charge, and their intensities depend on the temperature and Co and Ni concentration.

P.S.B.20.

FORMATION OF GAS PHASE CARBON AND NITROGEN CONTAINING MOLECULAR SPECIES AT HIGH TEMPERATURES

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Since 1989, when Liu and Cohen [1] predicted, based on the theoretical calculations, that "hypothetical covalent solids formed between carbon and nitrogen are good candidates for extreme hardness", carbon nitride solids, a new class of potentially super hard materials", have been the subject of considerable research efforts. The first synthesis of "covalent solid carbon nitride" [2] 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 synthesis is 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 different carbon and nitrogen containing species (CN, CN₂, C₂N, C₂N₂, C, C₂, C₃, N₂, N, etc.), but also the species containing hydrogen since the precursor molecules used sometimes in synthesis, contained hydrogen (C₃N₄H₄) too, at different temperatures. This process is investigated theoretically by computing the equilibrium composition of the gas mixtures containing nitrogen and carbon as well as the mixture of nitrogen, carbon with hydrogen. 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 bar and 5 bar.

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.

[1] Amu Y. Liu and Marvin. L. Cohen, *Science*, 245 (1989) 841.

[2] Chunming Niu, Yuan Z. Lu, Charles M. Lieber, . *Science*, 261 (1993) 334.

P.S.B.21.

RAMAN SPECTROSCOPY OF $Zn_{1-x}Mn_xGeAs_2$ CHALCOPYRITE

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We present Raman spectra of $Zn_{1-x}Mn_xGeAs_2$ semimagnetic semiconductor with the chemical composition $x \leq 0.185$. Our samples were previously characterized by X-ray diffraction, nuclear magnetic resonance and scanning electronic microscopy technique. The high field magnetoresistance show a presence of giant magnetoresistance effect. Raman spectrum of the undoped sample consists of 5 well resolved lines at 99 cm^{-1} , 167 cm^{-1} , 190 cm^{-1} , 213 cm^{-1} and 247 cm^{-1} . Mn doping influences the position and a broadening of those lines, as well as appearance of new lines at 108 cm^{-1} and at about 370 cm^{-1} . Registered phenomena are discussed in the frame of model for the phonons in multicomponent alloys.

P.S.B.22.

APPROACH TO MODELING INTERACTION OF CARBON FIBER MATERIALS AND LASER BEAM WITH EXPERIMENT

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During the interaction of material, built from carbon fiber, and laser beams come to a number of processes and effects on the exposed material. Methods for characterization, qualitative and quantitative description of these effects, are numerous. In this paper the treatment of selected material derived using alexandrite and other lasers, and the results were analyzed by SEM microscopy. Because of the complexity of the process, the interaction can't be described with a single approach. We used a thermal model and give an overview of other models (theory of fractals). Using the model can provide estimates of heat distribution in the material during the irradiation with laser beams. This is good base for prediction other processes in material, triggered by heating (e.g. photochemical processes). Surface oxidation is among the most interesting photochemical processes. Analysis of the images caused by the change deserves special discussion, which should be used for identification and interpretation induced processes.

P.S.B.23.

ELECTRON STRUCTURE OF THE NEW TERNARY INTERMETALLIC COMPOUNDS

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High-energy spectroscopy has been used to study the electron structure and valence state of new ternary intermetallic compounds, which crystallize in the ThCr₂Si₂ and CeNiSi₂ types. The compounds which crystallize in CeNiSi₂ types have low temperature Curie.

The calculations of electron energy bands E(k) and partial DOS for compounds were performed by the semi relativistic linear muffin-tin orbital method (LMTO) without considerations of spin-orbit interactions. Effective filling numbers of electrons in different bands of components in R.E.M₂X₂ (R.E. = Y, Sc; M= Fe, Co, Ni, Cu, Pd, Rh; X= P, Si, Sn, Sb) compounds have been calculated. On the basis of the obtained, photoelectron, X-ray emission spectra and calculation of density of total and partial electron states in R.E.M₂X₂ compounds, the localization of electron of s- and p-states of X has been established within the energy ranges 14-7 eV and 7-2 eV, respectively.

These states of X are hybridized with 4p-states of M atoms. The electron occupation of the d-states of the M atoms has a dominant influence on the degree of their hybridization. Between the experimental and calculated X-ray emission spectra R.E.M₂X₂ good agreement has been obtained.

P.S.B.24.

STRUCTURAL AND ELECTRICAL PROPERTIES OF BARIUM-ZINC-TITANATE CERAMICS SINTERED AT 1300°C

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The aim of this work was an investigation of structural and electrical properties of sintered barium-zinc-titanate ceramics. Mixtures of BaCO₃, ZnO and TiO₂ were mechanically activated in a planetary ball mill up to 80 minutes and sintered isothermally in air for 120 minutes at 1300°C. The phase composition in the BaCO₃-ZnO-TiO₂ system after milling and sintering was analyzed using the XRD method. The existence of pure barium-zinc-titanate has been registered. Microstructure analyses were performed using SEM. The results of electric resistivity, capacitance and loss tangent of the sintered samples were correlated with the XRD and SEM results.

P.S.B.25.

**ADVANCED CARBON NANOSTRUCTURES
FOR ADVANCED SUPERCAPACITORS**

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For definition of high-tech object as "advanced ..." both object and scope of its potential application should be clearly defined in terms of their characteristics and criteria. The criterial ultimate physical limit approach is applied to the case of nanostructures suited for double electric layer supercapacitors (SCs) based on advanced superionic conductors (AdSIC). These all solid state micron-sized SCs are required for the development of many high-tech directions. Ion-conducting nanostructures and devices are sure to play an important role in nanoelectronics and nanosystems which require the heterointegration of semiconductor devices, energy and power sources, sensors, actuators, etc. Nanoelectronics looks beyond the horizon of silicon integrated circuits, where prevalence may obtain the molecular or carbon electronics. In portable electronic based on surface mount devices (microSMD), capacitors are components of the largest size. Carbon-based (SCs) may be compatible with future carbon nanoelectronics. Within the context of a pointed problem, the question arises: is the reserve for significant improvement of the frequency-capacity and energy-power characteristics of carbon-based SCs? As an affirmative response on the question, the results of criterial ultimate physical limit approach for SCs are presented in this report. The consideration is performed in such term group as the densities of charge, current, energy, power, electrostatic capacitance, quantum capacitance, the maximal operational frequency of functional nanostructure, the voltage of electrochemical decomposition of ionic conductor/electronic conductor heterojunction, the crystal potential relief depth in an AdSIC. The cases of carbon based nanostructures suited for SC required for future deep-sub-voltage nanoelectronics are considered. The ways of increase of SC capacity density with use of graphene materials are offered. The uniform metal-covered carbon nanotubes, bundles of metal SWCNTs and graphene sheets with high concentrations of dopants and extended defects were proposed for the creation of high capacity advanced carbon electrode nanostructures for SCs. This work on the hetero-integration of semiconductor and nanoionic devices on the base of AdSIC is supported by the program 21 (Nanomaterials and Nanostructures) of the Presidium of Russian Academy of Sciences.

P.S.B.26.

**BINDING ENERGY OF HYDROGENIC IMPURITY
IN CdTe/ZnTe SPHERICAL QUANTUM DOT**

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Binding energy of a hydrogenic impurity located at the center of the CdTe/ZnTe spherical quantum dot has been calculated under the effective mass approximation by solving Schrödinger equation analytically. Eigenenergies are expressed in terms of the Whittaker function and Coulomb wave function. The results show that impurity binding energy strongly depends on QD size if it is less than an effective Bohr radius.

P.S.B.27.

**THE INFLUENCE OF BORON DOPING CONCENTRATION
ON MgH₂ ELECTRONIC STRUCTURE**

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We have performed *ab initio* electronic structure calculations of Mg_{1-x}B_xH₂ compounds with different boron concentrations, ranging from $x = 0.0625$ to 0.5. Full structural relaxation was performed in order to properly describe influence of dopant on host matrix. Results showed that there is a strong influence of dopant concentration on structural and consequently, thermodynamic stability of compound. B – H bond length is substantially shorter than in Mg-H coordination polyhedron, resulting in stronger and different kind of bonding. It is obvious that boron significantly contributes to density of states at Fermi level within energy gap. The width of boron electronic states heavily relies on boron concentration, causing reduction of energy gap of host MgH₂, and leading to metallic nature of compound with highest boron concentration. The predicted thermodynamic instability of compound with highest boron concentration is in agreement with experimental findings that under similar stoichiometry, boron with magnesium forms different hydride, Mg(BH₄)₂. Results also showed that existence of stable hydrides with MgH₂ rutile structure and small concentration of boron is possible and that boron can be used to further destabilize MgH₂ in order to enhance its hydrogen sorption-desorption kinetics.

P.S.B.28.

NANOCRYSTALLIZATION OF 30K₂O·30Nb₂O₅·40GeO₂ GLASS

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Developing techniques for fabricating nanostructures inexpensively is an area that requires substantial effort. Crystallization of glass is one of the effective methods for fabrication of nanostructures. Since glass crystallizes through nucleation and growth on heating, one of the key factors for nanocrystallization is the nucleation in glass. A structural similarity between glass and crystal should favour homogeneous nucleation. The glasses with the stoichiometric composition corresponding to a target crystal have a big chance for nanocrystallization. In this paper the crystallization of 30K₂O·30Nb₂O₅·40GeO₂ glass which composition corresponds to K₆Nb₆Ge₂O₂₆ crystalline phase was examined. The glass was melted in platinum crucible at T=1200 °C during t=1 h and its transition temperature $T_g=605^\circ\text{C}$ and crystallization peak temperature $T_p=657^\circ\text{C}$ were determined. The crystallization experiments were performed under isothermal conditions by heating a glass at 660-800 °C for t = 1-100 h. One and two-stage regimes of heating were employed. XRD analysis showed that this glass crystallized by the primary crystallization. As primary K_{3,8}Nb₅Ge₃O_{20,4} and K₆Nb₆Ge₂O₂₆ phases are formed, while K₁₀Nb₂₂Ge₄O₆₈, K₂NbO₃ and K₄Nb₆O₁₇ appeared as the secondary ones. The volume crystallization mechanism of these crystalline phases was detected. The size of crystals were in the range of 30-100 nm.

P.S.B.29.

TEXTILE DYE SORPTION BY POROUS AMINO FUNCTIONALIZED COPOLYMER

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Macroporous hydrophilic copolymers based on glycidyl methacrylate, GMA, proved very useful as sorbents and column packing in different types of chromatography, as enzyme supports, in biotechnological and biomedical applications, for heavy and precious metal sorption, the sorption of organic compounds, etc. In this paper, macroporous copolymer of GMA and ethylene glycol dimethacrylate, EGDMA, poly(GMA-co-EGDMA) [abbreviated PGME] was synthesized by suspension copolymerization. Copolymer was additionally functionalized via ring-opening reaction of the pendant epoxy groups with diethylene triamine [PGME-deta] and tested as acid textile dye sorbent.

The pore size distribution of PGME-deta was determined by mercury porosimetry (Carlo Erba 2000, software Milestone 200). The sorption experiments were carried out in thermostated shaker (Memmert WNE 14 and SV 1422). The samples were withdrawn from the shaker at regular time intervals and the dye solution was centrifuged. The absorbance of supernatant solution was measured. The spectra were obtained using Thermo Electron Nicolet Evolution 500 UV-VIS spectrophotometer and absorption peaks of acid dye was chosen for monitoring of sorption process.

The effect of pH and temperature on sorption efficiency of PGME-deta in removing textile dye from aqueous solutions was studied in order to evaluate this material as wastewater sorbent. Freundlich and Langmuir equations were used to determine the best fit model to correlate obtained experimental results. Kinetic data were treated with pseudo-first-order and pseudo-second-order kinetic models.

P.S.B.30.

**DETERMINATION OF POLY(VINYLPYRROLIDONE)
IN WASTEWATER AND RIVER WATER SAMPLES
BY CONTINUOUS FLOW OFF-LINE PYROLYSIS/GC-MS**

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In this work continuous flow off-line pyrolysis/gas chromatography-mass spectrometry (Py/GC-MS) was applied for detection and quantification of water-soluble polymer, poly(vinylpyrrolidone) (PVP), in wastewater and river water samples. The samples were pre-extracted with hexane and diethyl-ether, concentrated and pyrolyzed at 500 °C in order to cause rapid polymer fragmentation into volatile products – compounds capable of being analyzed using GC/MS. Continuous flow off-line pyrolysis coupled to GC/MS allowed a reliable quantification of PVP in complex environmental samples at trace levels. The concentrations of PVP were calculated on the basis on main degradation product, *N*-vinyl-2-pyrrolidone. The values of PVP in analyzed wastewater samples ranged from 0.9 to 7.1 mg/L, which represented an enormous contamination level. Also in affected river water samples very high concentrations of PVP of up to 180 mg/L have been detected. These results represent the first report of PVP contamination in the aquatic environment.

P.S.B.31.

**A KINETIC AND THERMODYNAMIC STUDY OF THE REMOVAL
OF AQUEOUS ZINC USING SERBIAN NATURAL CLINOPTILOLITE**

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Kinetic and thermodynamic aspects of the Zn²⁺ sorption on the Serbian clinoptilolite (from the Vranjska Banja mine) at different temperatures and different Zn²⁺ solution concentrations are reported. The sorption capacity of the clinoptilolite increases both with temperature and with the initial Zn(II) solution concentration. The sorption capacity at 298 K varies from 32% (for C₀= 100 mg Zn dm⁻³) to 64% (for C₀= 600 mg Zn dm⁻³). There is a roughly 1.4-fold increase in sorption capacity at 338 K: from 46% (for C₀= 100 mg Zn dm⁻³) to 92% (for C₀= 600 mg Zn dm⁻³). The sorption isotherm at 298-338 K is best represented by the Langmuir-Freundlich (Sips) model and the sorption kinetics by the pseudo-second-order model. The corresponding rate constant varies rather irregularly with temperature, the probable reason for this being a participation of diffusion and the presence of some complex zinc(II) species. The complex zinc(II) species could arise due to hydrolysis. The sorption involves a combination of three processes: the film diffusion, the intra-particle diffusion, and a chemical cation-exchange between the Na⁺ ions of clinoptilolite and the Zn²⁺ ions. The sorption is endothermic and spontaneous in the 298–338 K range. Thermal treatment of the Zn-loaded clinoptilolite leads to the formation of the nano-sized ZnO particles inside the lattice. The resulting system exhibits a moderate antibacterial activity towards Escherichia coli.

P.S.B.32.

**SAXS STUDY OF MICELLES AND NANOSTRUCTURED NETWORKS BASED ON
POLY(METHYL METHACRYLATE) / POLYHEDRAL OLIGOMERIC
SILSESQUIOXANE BLOCK COPOLYMERS**

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Structure of hybrid organic-inorganic nanostructured micellar and network systems based on poly(methyl methacrylate) / polyhedral oligomeric silsesquioxane block copolymers (P(MMA-co-GMA)-*b*-POSS,MA) was studied using Small-Angle X-Ray Scattering (SAXS). The micelles are formed by dissolving the block copolymer in a selective solvent. Effect of the solvent quality and the concentration, mass, composition and architecture of the copolymer on the micelle and network structures were investigated. A novel method to determine the molecular mass of nanoparticles, based on single SAXS curve in relative units, will be described.

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P.S.B.33.

THE INFLUENCE OF HARD SEGMENT CONTENT ON DYNAMIC MECHANICAL PROPERTIES OF SEGMENTED POLYURETHANES BASED ON POLYCARBONATE DIOLS

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Segmented polyurethane elastomers linear copolymers consisting of a relatively flexible component derived from a macrodiol, called the soft segment, and a relatively hard component derived from a diisocyanate and a chain extender, called the hard segment. In industry, considerable attentions have been devoted to new polycarbonate-based polyurethanes due to their improved mechanical and thermal performances compared to the traditional polyurethanes. The elastomeric materials based on polycarbonate diols are used for industrial parts, building materials, sports goods, medical equipment, and even artificial tissues due to their good biocompatibility. The goal of this work was to estimate the influence of hard segment content obtained by changing the ratio of OH group from diol and chain extender in the region from 0.5 to 10 for segmented polyurethanes obtained from hexamethylene-diisocyanate, polycarbonate diol and 1,4-butanediol as chain extender prepared in a bulk by one step procedure. The calculation of hard domains content was obtained by FTIR method and correlated with calculations based on reactive component content. Bands, characteristic for -N=C=O stretching region, were deconvoluted using Gaussian and Lorentzian curves, in order to get the information about the area assigned to hard segment content (from 15 to 41%). In an effort to assess the structure-properties relationships for prepared samples, dynamic mechanical measurements were performed. The glass transition temperature obtained from DMA measurements as a position of $\tan \delta$ maximum, was for all samples at about -31 °C, belonging to the soft segments of prepared thermoplastic polyurethane elastomers.

P.S.B.34.

**STRUCTURAL CHARACTERIZATION AND STATISTICAL PROPERTIES OF
TWO-DIMENSIONAL GRANULAR SYSTEMS DURING THE COMPACTION**

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The vibratory compaction of granular materials has long been of importance in technological applications. The underlying dynamic and structural properties of compaction process are a subject of great interest for physicists in recent years. The phenomenon of granular compaction involves the increase of the density of granular material subjected to shaking, tapping or, more generally, to some kind of external excitation. We study by numerical simulation the compaction dynamics of frictional hard disks in two dimensions, subjected to vertical shaking. Shaking is modeled by a series of vertical expansion of the disk packing, followed by dynamical recompression of the assembly under the action of gravity. The second phase of the shake cycle is based on an efficient event driven molecular dynamics algorithm. We investigate the compaction dynamics for various values of friction coefficient and coefficient of normal restitution. The granular organization at local level was studied by analyzing the shape factor ζ of the local volumes associated with a natural way of subdividing the volume into local parts—the Voronoi partition. The shape factor ζ is a quantifier of the circularity of Voronoi cells associated with the individual particles. It gives a clear physical picture of competition between less and more ordered domains of particles during compaction. We calculate the distribution of the shape-factor for packings at different stages of the compaction process. We have also investigated a two-dimensional granular medium experimentally (the motion of the grains is confined to a plane). We prepare granular packings of metallic cylinders of diameters 4, 5, and 6 mm. Experimentally, we focus our attention on the dependence of the microstructural properties of grains (grain displacement, Voronoi volumes) on some parameters like the packing fraction, and the effective gravitational field. We show, using a optical method developed experimentally, that the microscopic texture of the packing of grains is quite sensitive to the details of initial preparation of host granular packing such as mixture composition and initial packing fraction. The distributions of the shape-factor obtained numerically for various tapping intensities are consistent with our experimental results.

P.S.B.35.

TRANSPORT COEFFICIENTS IN MIXTURES $CF_4/Ar/O_2$ AND CF_2 OR F_2 RADICALS

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We present transport coefficients for electrons in mixtures of CF_4 with Ar and O_2 for ratios of the electric field to the gas number density E/N from 1 Td to 1000 Td ($1Td=10^{-21} Vm^2$). We then add a certain percentage of radicals CF_2 and F_2 produced by dissociation of CF_4 . Our analysis of non-conservative collisions revealed a range of E/N where electron attachment introduced by radicals significantly changes electron kinetics obtained for mixtures without dissociation of CF_4 gas. Results are obtained by using a simple, Two Term solutions for Boltzmann's equation but are verified by Monte Carlo simulations. It was found that three body attachments for oxygen is not significant for pressures that are standard in plasma etching equipment i.e. below 1 Torr. Furthermore it was found that attachment to CF_2 and F_2 at low mean energies is sufficient to change the nature of plasmas and turn them into ion-ion plasmas with very few electrons for realistic abundances. At the same time the mean energy and energy distribution functions are the same as in unperturbed gas mixture.

P.S.B.36.

PAIR INTERACTIONS IN TRANSITION METALS AT DIFFERENT ATOMIC DENSITIES

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At last years, nanoparticles of pure transition metals immobilized on the dielectric matrixes are widely used in different fields of advanced technologies: as carriers and transmitters of information, as an effective catalytic materials, *etc.* To understand this phenomenon it is necessary to study its nature on the microscopic level. From the theoretical point of view, the first steep of the understanding is construction of an effective pair interaction in the transition-metal nanoparticle. In general case, the d -electron contribution to the potential energy is non-pairwise. There are a number of approximated forms for the effective pair potential in the transition metal. Here, we use the Wills-Harrison approach based on the separate consideration of the d - and s -electron states. Effective pair potentials of the pure Fe, Co, and Ni are calculated at different atomic densities corresponding to liquid, crystalline, and nanocrystalline states. It is found that the minimum of the pair potential is deeper and oscillations are stronger in nanocrystalline state in comparison with the liquid and crystalline states for all metals under consideration.

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P.S.B.37.

CHARACTERIZATION OF NEW STRUCTURE FOR SILICON CARBIDE X-RAY DETECTOR BY METHOD MONTE CARLO

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This work presents an characterization of radiation absorption properties of silicon carbide (SiC) as semiconductor for the realization of detectors for X-rays. SiC detectors can potentially reach superior performance with respect to all the other semiconductors presently employed in hazardous environments in nuclear and space science and technology. Physics and numerical modelling of photons transport through SiC detector is incorporated in non-destructive Monte Carlo method for determining the energy deposited and dose distribution. The Monte Carlo code has been adopted for numerical simulations for different detector conditions and configurations. The X-ray characterization of new SiC structures originates the improving of design of these detector systems.

P.S.B.38.

COMPARATIVE STUDY OF HALOGEN ADSORPTION ON InAs(001) SURFACE

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The study of halogen adsorption on III-V semiconductor surfaces is very important from fundamental point of view and for technological application because they are very perspective reagent for making atomically abrupt structures. The mechanism of halogen (fluorine, chlorine and iodine) chemical bonding on the In-terminated ζ -InAs(001)-(4×2) surface was studied using ab-initio method within density-functional theory. The most stable adsorbate positions were determined. The electronic structure of new $\beta 3'$ -InAs(001)-(4×2) reconstruction is studied also. The microscopic nature of halogens interactions on both surface reconstructions is discussed. Various stable atomic configurations of halogens on the surface are considered in dependence on their concentration. The surface electronic properties are analyzed. It is shown that on both surface reconstruction halogens prefer to be bond with In dimer atoms. The interaction of halogens with surface dimerized atoms leads to weakening of chemical bonding between In and As surface atoms and determined the initial stage in the surface etching. The support of RFBR (grant № 09-02-01045a) and Program of SB RAS (interdisciplinary integration project N99) are acknowledged.

P.S.B.39.

ZnSiAs₂ AND ZnGeAs₂ ARE PERSPECTIVE MATERIALS FOR SPINTRONIC

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A^{II}B^{IV}C^V₂ chalcopyrites are electronic analog of A^{III}B^V compounds which are electronic analog of fourth group's semiconductors (Si, Ge). These compounds mostly have covalent type of chemical bond, small carrier effective mass, high carrier mobility and absolute minima and maxima of conduction and valence bands in the center of Brillouin zone.

The samples ZnSiAs₂<Mn> and ZnGeAs₂<Mn> were prepared like supersaturated solid solutions. The Curie temperatures of these compounds are 337 and 365K respectively. The magnetic properties of these compounds were explained by formation of nano-clusters MnAs. The sizes of magnetic clusters were calculated using relationships of superparamagnetism theory for the distribution function of the magnetic moment blocking temperatures. The average nanocluster size for ZnSiAs₂ increased from 3.1 to 3.6 nm as the manganese level in ZnSiAs₂ increased from 1 to 2 wt.%.

The difference between lattices ZnGeAs₂ and GaAs is less than 2%, this provide good conditions for epitaxy. ZnSiAs₂ is structurally compatible with silicon. Using the phase diagram Si-ZnAs₂ through reaction ZnAs₂ with silicon substrate was getting thin film ZnSiAs₂ with manganese. The magnetic properties of the film ZnSiAs₂<Mn> was the same like for bulk crystals.

ZnSiAs₂ and ZnGeAs₂ with manganese doped are perspective materials for spintronic because they have Curie point above room temperature and they are structurally compatible with Si and GaAs respectively. It let us think what these compounds can be used for spintronic's modern devices.

P.S.B.40.

THERMODYNAMIC CHARACTERISTICS OF ONE-DIMENSIONAL STRUCTURES

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One-dymensional crystal lattice with single atom per unit cell is analysed in the nearest neighbour harmonic approximation. Thermodynamic functions (specific heat and thermal conductivity) are numerically calculated in the wide temperature range by using exactly known phonon density of states and Calaway model for thermal conductivity. In extreme cases of low and high temperatures these thermodynamic functions are found in analytical form. For thermal conductivity the results of Calaway model for exact phonon density of states are compared with the results of Calaway model for Debay approximation of phonon density of states.

P.S.B.41.

OPTICAL SPECIFICITY OF ULTRATHIN CRYSTALLINE FILMS

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The changes of optical properties under boundary presence in molecular crystal nanofilm were theoretically investigated in this work. The dispersion law and 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.42.

THE LOW POWER LIGHT EMITTING DIODE PHOTOACOUSTIC

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The various types and applications of photoacoustic techniques have generally enjoyed steady growth in the recent thirty years because these techniques allow the obtaining information about nanostructure materials that is often not obtainable using more traditional method. We have developed the novel photoacoustic system using a light emitting diode (LED) light source with monotone modulation of intensity, the photoacoustic cell, and microphone and developing the digital lock-in amplifier especially customized for low power photoacoustic gas-microphone detection, acquisition system and theoretical models with software, enabling realization of various typical and user defined analysis that contributes in determination of sample properties. The reliability, sensitivity and selectivity of the instrument have been compared with ones of the conventional photoacoustic setting that uses commercial lock-in amplifier and the same other element of the experimental setup. The capability of the developed instrument to give some new informations about solids and to be extended in the photoacoustic and photothermal laboratory controlled by PC is discussed.

P.S.B.43.

**COMPARATIVE ANALYSIS OF NEW SENSING MATERIALS
IN CHEMICAL SAW SENSORS**

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Comparative analysis of different, new gas sensing materials in surface acoustic wave (SAW) chemical sensors is presented. Different gas sensing materials as polyaniline, teflon AF2400, polyisobutylene (PIB), Co-tetra-phenyl-porphyrin, polyepichlorohydrin (PECH) are considered. In the analysis the new method of the complete analyses of gas chemical sensors is used. The method is based on the electromechanical equivalent circuit of the SAW sensor. The method is very efficient and can be used for the optimal design of CO₂ sensors. The results are compared with results presented in open literature.

P.S.B.44.

**AN ADVANCED SURFACE POTENTIAL MODEL OF MOS INVERSION LAYER
INCORPORATING THE QUANTUM MECHANICAL EFFECTS**

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Significant quantum mechanical effects, primarily caused by the high substrate doping and small effective oxide thickness, occur in the actual MOS transistors. These two factors often cause severe band bending on the Si side of the Si-SiO₂ interface, due to the very high electric field which is present here. The resulting potential well becomes narrow enough to cause significant energy quantization of the carriers in the direction perpendicular to the interface. In this case, the conduction band can no longer be regarded as a continuum of states, but rather splits into discrete subbands. All of models which take into account quantum mechanical effects are based on coupled Poisson's and Schrodinger's equations which can be solved using numerical simulations obtained from a self-consistent Poisson-Schrodinger solver for a wide range of substrate doping and oxide thickness, or by using a variational wave function approach. The compact MOS transistor models used for circuits simulation need to incorporate the quantum mechanical effects in an approximate and efficient manner. In order to obtain satisfactory results, a number of researchers have worked on developing appropriate approximation of surface potential MOS inversion layer model based on well-known implicit relation. This relation can be solved numerically, incurring expensive computation time. To overcome this difficulty, several solutions have been proposed for obtaining an explicit approximate relation for surface potential as a function of terminal voltage. In this paper an approximate description of surface potential model, which include a quantum mechanical correction, will be developed. These solutions, which are explicit and analytical, are based on smoothing functions and parameters so that physical approximate expressions could be available in the weak and strong inversion. The smoothing functions of different forms are used and their availability is analyzed by comparison with results obtained using self-consistent Poisson-Schrodinger solver. The comparison with numerical data shows that the solution gives an accurate approximation of surface potential for nanoscale MOS transistors in all regions of operation.

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P.S.B.45.

μ SR ON CeCo₄B UNDER PRESSURE

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Polycrystalline CeCo₄B was prepared by arc melting the constituent elements in argon atmosphere. The sample crystal structure was checked by X-ray measurements and was found to be single phase. Magnetic properties of the sample were studied in the temperature range 4.2-850 K and external magnetic fields up to 12 T. μ SR measurements were performed at different pressures in the range of 0-9.5kbar.

From the μ SR measurements at the ambient pressure the temperature dependence of the order parameter in CeCo₄B compound was obtained. In the same time the transition temperature, ($T_c=293$ K) from ferrimagnetic order to paramagnetic behavior was determined. The analysis of the experimental results around the structural temperature transition T_t , suggests that the transition is not a pure structural transition, being accompanied by a sublattice magnetization reorientation.

The anomalies, observed in macroscopic measurements at T_t are enhanced by the applied pressure and shifted to larger temperatures while T_c is reduced. The order parameter and the transition temperatures decrease when the pressure increases while the structural/reorientation transition temperature increase with increasing pressure. This behavior was explained by considering the enhancement of (4f+5d)-3d hybridization due to the decrease of the interatomic distances with increasing pressure.

P.S.B.46.

THERMAL MEMORY PROPERTIES AND DEPTH INHOMOGENEITY OF POLYOLEFINES DETERMINED BY THE PHOTOACOUSTIC FREQUENCY METHOD

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In this article, we present a short review of the recent development of the theoretical model for the gas-microphone photoacoustic, including thermal memory effects and thermal depth inhomogeneity of a thin sample. Measuring of the thermal relaxation time and depth profile of thermal diffusivity of polyolefines is based on the aforementioned model and conducted on the recently developed experimental apparatus. The obtained result is very important since it represents the first measurement of thermal memory properties in the world and their recognition is significant not only for employing of conventional polyolefines in modern applications, but also for further fundamental research.

P.S.B.47.

EXPLORATION OF LASER INTERACTION WITH FERROMAGNETIC SHAPE MEMORY ALLOYS

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Shape memory alloy joining can be a difficult task, especially since it involves materials that are affected by heat dissipation in the joining area. Laser welding can be a solution for joining shape memory alloys, but its influence on ferromagnetic shape memory materials has not been explored so far. Our experiments have been performed on several alloy families with the aim to understand the influence of the laser interaction with the materials, in order to assess the use of this type of joining in future potential applications. Microstructural investigations are comparatively performed on the base material, melted and heat affected zone and discussed in relationship with specifics of the ferromagnetic shape memory alloy family.

P.S.B.48.

PLASTICALLY DEFORMED $Ti_{50}Ni_{25}Cu_{25}$ SHAPE MEMORY ALLOY RIBBONS

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Crystallographic particularities play a key role in the occurrence of the shape memory and associated properties. Plastic deformation can be a practical tool to further control the crystallinity of shape memory alloys produced by rapid solidification. Shape memory alloy ribbons have been manufactured by melt-spinning and experiments were performed on rolled and stack-rolled $Ti_{50}Ni_{25}Cu_{25}$ shape memory alloy ribbons with the aim to explore the resulting effect on the microstructural and functional properties. The plastic deformation ranged from 40% to 60% in single or multiple steps. The structure of the ribbons was examined using optical and electron microscopy and simultaneous X-ray diffraction and electric resistance measurements.

P.S.B.49.

THE INFLUENCE OF STRONTIUM ON POROSITY FORMATION IN Al-Si ALLOYS

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Strontium modification is known to alter the amount, characteristics and distribution of porosity in Al-Si castings. Strontium is added to hypoeutectic aluminium-silicon alloys in order to transform the morphology of the eutectic silicon from faceted acicular flakes to a fibrous rodlike form, thereby improving mechanical properties. Sand –cast plates of six compositions were produced in order to determine the effect of strontium addition on porosity formation in Al-Si alloys. Strontium has been shown to modify the eutectic and change the eutectic solidification mode in Al-Si alloys over the entire range of strontium addition. The addition of strontium reduced porosity in the hot spot region of the casting, and the pores became well dispersed and rounded. The results of the experimental work were analyzed using statistical techniques to determine the validity of trends identified in the data because of the limited experimental data. The analysis of the results showed that addition of strontium altered the amount, distribution and morphology of the porosity in the alloy with a large volume fraction of eutectic. No apparent differences in the amount, distribution and morphology of the porosity were observed between strontium free and strontium containing alloys with no or very small eutectic volume fractions. This results can be explained by considering the combined effect of the casting design and the differences in the pattern of eutectic solidification between unmodified and Sr – modified alloys.

P.S.B.50.

MECHANICAL AND TERMOMECHANICAL LASER TREATMENT OF IRON BASE SUPERALLOY N – 155

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Iron base superalloy N – 155 samples were cut from the turbine blade after longtime service at elevated temperature and pressure. The samples were exposed to mechanical and thermomechanical laser treatment, and observed by scanning electron microscope (SEM) and analyzed by energo-dispersive spectrometry (EDS). Also, the samples were cold rolled, laser treated and microstructural changes were discussed. Further, the cold rolled samples were exposed to aggressive medium, laser treated and analyzed by SEM and EDS, as well. Vickers microhardness tests were performed. In this paper, microstructures arising after these three different conditions of investigation were analyzed and compared.

P.S.B.51.

**MICROSTRUCTURAL CHANGES ARISEN BY INTERACTION
OF PICOSECOND LASER WITH AUSTENITIC MATERIALS**

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Investigation was carried out on austenitic material samples – stainless steel and iron base superalloy that are widely used at elevated temperatures and pressures. The samples were exposed to Nd:YAG pulsed laser, with wavelength of 1064nm and pulse duration of 170 ps. Different pulse energy and number of pulses were applied. Spots obtained by laser interaction were observed by optical and scanning electron microscope and analyzed by ergo-dispersive spectroscopy. Vickers microhardness tests were performed. In this paper, the microstructural changes, arisen by different pulse energy and number of pulses, were discussed with the aim to determine optimal laser parameters in surface treatment process.

P.S.B.52.

MICROSTRUCTURE AND PROPERTIES OF CMnSiMo STEEL UPON Q-P PROCESS

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An excellent combination of tensile strength and elongation is the most important factor in design of new heat treatment procedures of low alloyed steels. Among advanced heat treatment processes capable of reaching this goal there is also the Q-P process (Quenching and Partitioning), where the final material properties are given through combination of martensite and very fine retained austenite. Experiments with CMnSiMo steel with enhanced molybdenum content have been performed. Considering the fact that molybdenum leads to stabilizing of austenite and deceleration of precipitation kinetics, this alloying concept is expected to bring very good mechanical properties. The paper is aimed at testing the influence of the Q-P process on evolution of final microstructure and mechanical properties of the CMnSiMo steel.

P.S.B.53.

APPLICATION OF THERMOGRAPHY FOR EVALUATION OF TENSILE PROPERTIES OF MATERIALS AND WELDED JOINTS

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This paper presents experimental results of comparative tensile tests of base material and butt welded joints (S355J2G3) by use of thermography and standard methods. During tensile testing deformation of base and weld material is occurring. The appearance of plastic deformation is accompanied with the temperature increase in the zone where plastic deformation is present. Test specimens are tested on electro mechanical tensile testing machine with the application of the control strain. These tests have shown the potential for application of non-contact thermography during deformation of material where possibility for prediction of damage in welded structures and materials exists.

P.S.B.54.

INFLUENCE OF HEAT TREATMENT ON CORROSION BEHAVIOUR OF MAGNESIUM ALLOY AZ61 IN ARTIFICIAL ATMOSPHERE

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The influence of heat treatment on microstructure and corrosion behaviour of AZ61 exposed to salt spray was evaluated. Experimental material was manufactured by a squeeze casting process. Specimens for salt spray testing were as fabricated and solution heat treated (380°C). Heat treating time was chosen in consideration of remaining aluminium segregation after solution treating. Chemical and structural heterogeneity were characterized by scanning electron microscope (SEM) and scanning electrochemical potential microscope (SECPM). Corrosion rates of as cast a heat treated material were compared to determine the influence of alloy microstructure a chemical heterogeneity on corrosion degradation.

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P.S.B.55.

**VIDEOEXTENSOMETRIC AND HV 10 MEASURING
OF DEFORMATION PROCESSES IN AUTOMOTIVE STEEL SHEETS**

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Videotensometry measuring is non contact sensing deformation of plane samples. The samples IF - steel, DP - steel and microalloyed steels was determined longitudinal deformation at different notch and without notched. We determined the relationship between deformation and hardness HV 10. Samples were taken with videotensometry scanning techniques using CCD camera, resulting in the deformation maps of Matlab. The samples after rupture was measured hardness HV 10. Hardness HV 10 is grown with plastic deformation steels.

This study was supported by the Grand Agency of Slovak Republic, grand project APVV No. 0326-07.

P.S.B.56.

**THE ROLE OF HEAT TREATMENT PROCESS ON THE CHARACTERISTICS
OF CONNECTION Al-Si12CuNiMg**

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Pistons of engines marine vessels are important details, that work in difficult working conditions, therefore the selection process of material and processing technology is devoted to the special importance. In this study for the silumin connection Al-Si12CuNiMg, based on a series of experimental tests, were given parameters of the process of thermal processing, temperature, time to the hardening process and wear. Research and experimental work is based on better recognition of the technological characteristics of spill process, and the role of connecting chemical elements on mechanical and structural characteristics. The results obtained were accompanied by definition of mechanical properties (strengths), physical (linear expansion), as well as estimates of comparative microstructure and electron-structure. From the results obtained, it turned out that the cycle that gives the highest properties, is that of hardening in water with a temperature of 50°C after six hours at 510°C and that of further wear for 2 hours at 210°C.

Keywords: Pistons, thermal processing, silumin connections, hardening, temperature, temperature of wear.

P.S.B.57.

**MONITORING OF EXTERNAL APPAREL CONSUMER OF MARINE VESSELS
THROUGH THE NO DEVASTATING METHOD WITH ULTRASONIC**

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Outer coating of marine vessels is an important part of the ship that ensures reliability and quality of services to maritime transportation. On life of outer coating often were defined the costs of shipping services. The insurance of boat requests was reached not only during the design phase but also during their use in its periodic monitoring. Today there are many methods of monitoring, but in this study, monitoring was realized through the use of ultrasonic techniques. The portable equipment for measuring the consumption of boat, which is used, function on the basis of a sensor that produces a sound pulse that passes through the layer of steel and thanks to a chip stores (memorize) the time that takes the sound to be overwhelmed the thickness of sheet steel. On these results appears in the display of calibrated equipment the thickness of the layer.

Keywords: monitoring, ship, consumption of the boat, the ultrasonic, non devastating methods.

P.S.B.58.

DETERMINATION OF THE EFFECTIVE DIFFUSION COEFFICIENTE

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The equation for drying kinetics is obtained, based on the analytical solution of the differential equation with a boundary condition in the form of the flux. This equation was firstly developed by G. Efremov. In this paper it will be presented a modification of the Efremov drying equation. Shrinkage correction will be included in that equation for the first time. Software for determination of the effective diffusion coefficient is design and the predicted value fits well with the experimental data.

Key words: effective diffusion coefficiente, analytical solution, software.

P.S.C.1.

MECHANOSYNTHESIZED Ca_2SnO_4 AND Zn_2SnO_4 : NONEQUILIBRIUM NANOSTRUCTURE AND ELECTROCHEMICAL PERFORMANCE

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Nanostructured stannates, Ca_2SnO_4 and Zn_2SnO_4 , with an average particle size of about 15 nm were synthesized via single-step mechanochemical processing of binary oxide precursors at room temperature. A nonuniform structure of the mechanothesized stannate nanoparticles, consisting of an ordered core surrounded by a disordered surface shell/interface region, is visualized using HR-TEM. Solid-state ^{119}Sn MAS NMR and ^{119}Sn Mössbauer spectroscopy revealed a nonequilibrium nanostructure of the stannates characterized by the deformed SnO_6 octahedra. XPS was used to study the near-surface layers of the as-prepared nanoparticles. Nanosized Ca_2SnO_4 and Zn_2SnO_4 were tested electrochemically as anode materials for Li-ion batteries.

P.S.C.2.

AGING AND MEMORY EFFECTS IN INTERACTING NANOPARTICLE SYSTEM $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ OBTAINED BY A MECHANOCHEMICAL SYNTHESIS

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Nanoparticle $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ with crystallite size of 9 nm was obtained by a mechanochemical synthesis. This system represents concentrated magnetic nanoparticle system, where each particle possesses magnetic moment (superspin) which interacts with neighbouring moments. In this sense, the system is very good candidate for research on collective spin dynamics and spin glass characteristics. Obtained frequency dependence of AC susceptibility maxima, which can be fitted to the power-law form for the critical slowing down, represents clear indication of spin glass behavior. Zero-field-cooled measurements showed pronounced $M(T)-M_{\text{ref}}(T)$ dip around the waiting temperature pointing to the existence of a memory effect. This dip is proportional to the waiting time and speaks in favour of the presence of strong interparticle interactions i.e. collective dynamics. Aging effect was investigated by $M(t)$ relaxation measurements that were performed at different temperatures. At all measured temperatures, pronounce dependence on waiting time t_w is observed while relaxation rates S show maxima at the observation times close to t_w . All these features are entirely due to the collective dynamics, which is the consequence of the strong dipolar interactions among superspins in nanoparticle $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$.

P.S.C.3.

**MAGNETIC BEHAVIOUR OF NANOPARTICLE $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$
OBTAINED BY A MECHANOCHEMICAL SYNTHESIS**

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Single-phase perovskite compound $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ was synthesized by a high-energy ball milling in a single step processing. Structure and morphology characterizations revealed nanoparticle nature of this mixed valent manganite with the average particle diameter of 9 nm. Comprehensive set of magnetic measurements showed that the system can be described as an ensemble of interacting magnetic nanoparticles where each particle possesses high magnetic moment, i.e. superspin. Furthermore, magnetic behavior showed contributions from both superspin-glass (SSG) and superparamagnetic (SP) states, and the prevailing properties depended on the experimental conditions. It was established that SSG state dominated in low magnetic fields up to 500 Oe while in higher applied fields suppression of collective behavior occurred, and so individual characteristics of nanoparticles prevailed. It was also concluded that the applied method of synthesis produced system with high magnetic anisotropy as well as with the large nanoparticle shell whose thickness amounts 30% of a particle diameter.

P.S.C.4.

**INFLUENCE OF MILLING PARAMETERS ON PROPERTIES
OF $\alpha\text{-Al}_2\text{O}_3$ NANOPOWDER**

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The effect of experimental conditions on properties of mechanochemically produced nano-alumina powders has been studied. It was noticed that the relative humidity (RH) of surrounding gas media during grinding exerts a strong influence on the medium particle size and the degree of agglomeration of the powder produced. A pronounced minimum of the size of the resulted particles has been obtained at RH value close to 1%. Relations between properties of the powder stipulated by parameters of mechanochemical activator performance and densities of sintered compacts have been analyzed. The dependence of final density (more than 98% of theoretical value) on the intensity of milling presents a curve with an extremity. Reasons that are supposedly responsible for the extreme character of the dependences have been considered. Experimental data has been obtained with the aim of X-ray, SEM, BET, DLS etc. procedures.

P.S.C.5.

**AMINO-FUNCTIONALIZED CARBON NANOTUBES AS SUPPORT
FOR Pt NANOCATALYST**

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Multi-walled carbon nanotubes (CNTs) were used as a supporting material for Pt nanoparticles prepared by the microwave-assisted polyol method. The CNTs were pretreated by the chemical oxidation (o-MWCNT) followed by the modification by ethylenediamine (e-MWCNT). The Pt loading of Pt/o-MWCNT was only 2 mass % while the loading of Pt/e-MWCNT was 20 mass%. The investigation by transmission electron microscopy revealed that the mean diameter of Pt particles in Pt/e-MWCNT is 2.5 ± 0.5 nm and that their distribution on the support is homogenous with no evidence of pronounced particles agglomeration. Cyclic voltammetry of Pt/e-MWCNT thin film indicated clean Pt surface with well-resolved peaks characteristic for polycrystalline Pt.

P.S.C.6.

**INFLUENCE OF HEATING RATE ON TWO-STEP SINTERING BEHAVIOUR
OF DIFFERENT HYDROXYAPATITE NANOPOWDERS**

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Producing of dense nanostructured calcium phosphate-based bioceramics represents a challenging issue in biomaterial science. High volume fraction of energetically rich grain boundaries contributes to improved attachment of chemical species, which are important in the processes of bone tissue regeneration. Beside that, nanostructured ceramics exhibited better mechanical properties due to changed fracture path. The process of pressureless sintering is the most compatible route for industrial fabrication of dense bioceramic materials, but it is often connected with accelerated grain growth in final sintering stage. In the method of two-step sintering (TSS) the difference between kinetics of grain boundary diffusion and grain boundary migration is used to obtain almost full dense, nanostructured ceramics. However, designing of proper sintering parameters is very important in every sintering technique employed.

In this study, hydroxyapatite nanopowders were synthesized by different methods, precisely, chemical precipitation and hydrothermal processing of precipitate. The prepared powders were pressed in pellets and heated with different heating rates (2, 5, 10 °C/min), with short isothermal dwell at certain temperature range. From that shrinkage curves the appropriate conditions were selected to design TSS experiments. The impact of heating rate on final density, phase composition, average grain size and microstructural uniformity is discussed. Furthermore, mechanical properties were determined.

P.S.C.7.

**OPTICAL PROPERTIES OF SILVER NANOPARTICLES
IN NONPOLAR ORGANIC SOLVENTS**

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In order to develop method to synthesis silver nanoparticles different sizes, reaction between the silver salt and oleylamine in nonpolar organic solvents has been investigated. The silver organosols display several advantages over other silver hydrosols, such as the ability to be isolated and redissolved in solvents without irreversible aggregation, stability to air, and so forth. By changing the growth temperature, solvents and time of reaction, silver nanoparticles different sizes were produced (7-25 nm). The three solvents (chloroform, hexane, dichlorobenzene) were chosen. The influence of size and dielectric property of surrounding media on surface plasmon absorption band of silver nanoparticles are discussed. The average size and particle size distribution of silver nanoparticles was determined using transmission electron microscopy. The obtained silver organosols were optically characterized using UV-Vis spectroscopy. The advantages of such a method can be found in the applications of metal nanoparticles as catalysts and has been successfully extended to synthesis of other metallic colloid such as gold and copper.

P.S.C.8.

PHOTOLUMINESCENCE PROPERTIES OF Eu^{3+} DOPED TiO_2 NANORODS

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Hydrothermal treatment (90min/250°C) of suspension of scrolled titania nanotubes in the presence of $\text{Eu}(\text{NO}_3)_3$ and in the mild acidic conditions (pH~5-6), was used for the synthesis of Eu^{3+} doped TiO_2 nanorods. Nanorods were doped with two different concentrations of Eu^{3+} ions. Size and shape of titania nanotubes and Eu^{3+} doped titania nanorods were determined by TEM analysis. Postsynthetic treatments of doped nanorods by filtration or dialysis against water (pH~5-6) for three days at 4°C were applied with aim to remove excess of dopant ions from surface and to investigate the influence of their position on photoluminescence spectra. Eu^{3+} ions occupy two different sites of titania nanorods having different binding energies: core octahedral sites and undercoordinated surface sites. Photoluminescence spectra of Eu^{3+} doped TiO_2 nanorods independently of dopant concentration consist of three characteristic emission peaks located at $\lambda=544$, 596, and 617 nm that are attributed to the intra-4f transitions of Eu^{3+} ions, actually ${}^5\text{D}_1 \rightarrow {}^7\text{F}_0$, ${}^5\text{D}_0 \rightarrow {}^7\text{F}_1$ and ${}^5\text{D}_0 \rightarrow {}^7\text{F}_2$ transitions, respectively. Removal of Eu^{3+} ions from undercoordinated surface sites with lower symmetry applying postsynthetic treatment of suspension of Eu^{3+} doped TiO_2 nanorods (dialysis against water) caused change in photoluminescence spectrum. Namely, the intensity of the hypersensitive forced electric-dipole ${}^5\text{D}_0 \rightarrow {}^7\text{F}_2$ transition decreases in dialyzed samples, inducing the decrease in intensity of peak at $\lambda=617\text{nm}$ in photoluminescence spectrum. Elimination of excess of Eu^{3+} ions and Eu^{3+} ions from low symmetry surface sites, leaving only those located in the Ti^{4+} lattice sites with octahedral symmetry, simply applying postsynthetic treatment on Eu^{3+} doped TiO_2 nanorods open up possibility to manipulate the dopant position.

P.S.C.9.

SYNTHESIS OF LUMINESCENT ROD-LIKE ZINC TUNGSTATE NANOPARTICLES BY REFLUX METHOD

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Zinc tungstate (ZnWO_4) rod-like nanoparticles with *length* smaller than 10 nm, were synthesized for the first time by reflux method at 95°C for different reaction time in the presence of non-ionic copolymer surfactant. The structural characterization of the ZnWO_4 nanoparticles was performed using transmission electron microscopy (TEM) and X-ray diffraction (XRD) analysis. The XRD results indicated that as-synthesized rod-like nanoparticles exhibited only wolframite structure ZnWO_4 without impurities. The average crystalline domain size was estimated using the Debye - Scherrer diffraction formula. The grain size was found to be about 8 nm. Two emission bands in the UV and visible regions were observed. The UV narrow band with a peak wavelength of approximate 375 nm and a visible bluish-green emission with a peak at 460 nm were observed. Based on *diffuse reflectance spectra* the band gap was estimated to be 3.67 eV for synthesized nanoparticles of ZnWO_4 .

P.S.C.10.

SOLVOTHERMAL SYNTHESIS OF EuO NANOPARTICLES

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EuO attracts attention of scientists due to combination of magnetic and semiconductor properties it possesses. In the present work we propose a novel solvothermal method of EuO colloidal solutions synthesis based on europium compounds solvolysis in high-boiling solvents at relatively high temperatures (150–200°C) in presence of surfactants (oleylamine, oleic acid). TEM study showed that synthesized at 175–225°C colloids consisted of 1-5 nm particles and increase in synthesis temperature lead to simultaneous increase in average particle size. Electron diffraction data obtained for all colloids synthesized corresponds well with PDF#18-507 clearly showing that all colloids contain EuO nanoparticles. The work was supported by RFBR (grants # 10-03-01187, 09-03-12191-ofi-m and 09-03-01067) and FEA (grant P1214).

P.S.C.11.

SYLILATION OF MONTMORILLONITES TO INCREASE COMPATIBILITY WITH PMMA

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In this work the organo-silylations of a sodium montmorillonite and of an alkyl ammonium modified montmorillonite are realized and PMMA nanocomposites by in situ polymerization are prepared.

Silylated MMT has been characterized by FT-IR analysis and contact angle measurements. The SEM images of nanocomposites fractured surface show the absence of clays aggregates, confirming a good dispersion and distribution of MMTs in polymer matrix.

All nanocomposites present improved thermal properties. However the best results are obtained in presence of silylated montmorillonites, clearly the organosilane improves the compatibility between polymer matrix and clay and as effect the properties of nanocomposites.

P.S.C.12.

**EVOLUTION OF POLYANILINE 12-TUNGSTOPHOSPHATE
MICRO/NANOSTRUCTURES**

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Polyaniline 12-tungstophosphate (PANI-WPA) micro/nanostructures were synthesized by the oxidative polymerization of aniline in aqueous solutions of 12-tungstophosphoric acid. Non-conducting submicro-/microspheres, isolated after the first exothermic phase of polymerization, contain oligoaniline intermediates and incorporated 12-tungstophosphate ions. Semiconducting PANI-WPA, isolated after the second exothermic phase, consists of nanotubes and/or nanorods which coexist with submicro-/microspheres. The evolution of molecular, supramolecular and crystalline structure of polymerization products during a single polymerization process is studied by FTIR, Raman and inductively coupled plasma optical emission (ICP-OES) spectroscopies, elemental analysis, scanning and transmission electron microscopies (SEM and TEM), thermogravimetric analysis (TGA), differential thermal analysis (DTA), and X-ray powder diffraction (XRPD).

P.S.C.13.

**OXIDATION OF ANILINE WITH PEROXYDISULFATE IN THE PRESENCE
OF TANNIC ACID: POLYANILINE MICRO/NANOSTRUCTURES**

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Aniline has been oxidized with ammonium peroxydisulfate (APS) in aqueous solutions of tannic acid (TA). The effect of initial mole ratios [TA]/[aniline] and [APS]/[aniline] on the morphology and molecular structure of synthesized polyaniline tannate (PANI-TA) was studied by scanning (SEM) and transmission (TEM) electron microscopies, and FTIR and Raman spectroscopies. Optimum conditions for the preparation of PANI-TA with prevalent morphology of nanorods (an average diameter ~70–100 nm), and PANI-TA consisting of solely solid microspheres (an average diameter 0.8–3.5 μm) were found. The PANI-TA nanorods exhibit electrical conductivity of $\sim 10^{-3}$ S cm⁻¹, while the PANI-TA microspheres are nonconducting.

P.S.C.14.

SYNTHESIS AND CHARACTERIZATION OF NANOSTRUCTURED TRANSITION ALUMINA WITH HIGH SURFACE AREA

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Transition phases of alumina are metastable polymorphs of aluminum oxide formed through the thermal dehydration of aluminum trihydroxide (bayerite and gibbsite) and aluminum oxyhydroxide (boehmite). Transition aluminas, such are γ and η alumina with high surface area have very broad possibilities of application in ceramic industry, in catalysis, as adsorbents, biomaterial, reinforcement materials of metal–matrix composites etc. The main subject of this work was to elucidate conditions of preparing the transition alumina nanopowders with high surface area, starting from sodium aluminate solution obtained from Bayer process. Starting solution was neutralized by sulfuric acid and depending on the conditions of this process aluminum hydroxide, AH, or aluminium oxhydroxide, AOH, nanopowders (boehmite, pseudoboehmite, bayerite or gibbsite) were obtained. The other group of samples was synthesized by adding glucose and oxalic acid to the Bayer liquor for increasing surface area and creating mesoporous structure of alumina. All powders AH and AOH powders were dried at 100°C in air to remove water and other volatiles and after that samples heat treated up to 500°C, for a different time. The powders were characterized using: FT-IR spectroscopy, BET, DTA/TG, XRD, SEM and DLS method. Obtained results confirmed that all samples are nanostructured with average particle size less than 25 nm. The phase composition of nanostructured alumina depends on the composition of the starting powder and results have confirmed that bayerite as starting powder is favorable for obtaining η -phase with high surface area (374 m²/g) even without glucose, but with wide pore distribution. The glucose has more pronounced effect on increasing surface area of transition alumina in respect to oxalic acid (which was up to 500 m²/g). In addition glucose had an effect on narrowing the pore size distribution, where the mean size was approximately 5 nm.

P.S.C.15.

**THE INFLUENCE OF In^{3+} AND Y^{3+} IONS ON STRUCTURE
AND MAGNETIC PROPERTIES OF NANOCRYSTALLINE ZnFe_2O_4**

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The fascinating structural, magnetic and electronic behaviour of ferrite compounds have long been of interest to solid state scientists. These materials exhibit a complex relationship between preparation method, form (single-, poly- or nano-crystalline), composition, crystal structure and physical properties. We present here the results of the investigation of the structural and magnetic properties of nanostructured zinc ferrites, ZnFe_2O_4 and zinc ferrites substituted with indium and yttrium, $\text{Zn}_{0.85}\text{In}_{0.15}\text{Fe}_2\text{O}_4$ and $\text{ZnY}_{0.15}\text{Fe}_{1.85}\text{O}_4$. Powders based on zinc ferrites were synthesized by a coprecipitation method. The results of X-ray and TEM analyses confirmed the nanosized nature and spinel type structure of the investigated samples. Mössbauer spectroscopy studies revealed that there is a disorder among the cations between tetrahedral and octahedral sites in the spinel structure. The study of the magnetic properties showed that hysteresis loops do not saturate even in the presence of high magnetic fields, which confirmed the superparamagnetic and single domain nature of the samples. Addition of indium results in a decrease of the particle size and magnetisation and increase of coercivity of the nanoparticles. Yttrium has an opposite effect. This observation implies that, besides size, composition causes also significant structural rearrangements which in turn induce changes in magnetic behavior of the investigated nanoparticulate systems.

P.S.C.16.

NANOSTRUCTURED RELIEF TO ORIENT LIQUID CRYSTALS MATERIALS

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Electrooptical nematic liquid crystal (LC) cells, which can be used as laser switching devices, electrically and optically addressed spatial light modulators, and analogs of display elements, mostly operate in *S* and *T* configurations, which realize a planar orientation of the LC mesophase on the aligning substrate surface. However, the solution of some problems, where the initial black field is necessary for the regime of light transmission through the cell structure, requires a homeotropic alignment of LC molecules on the substrate. In the present paper the possibility of obtaining homeotropic orientation in thin_film nematic liquid crystal cells using carbon nanotubes is considered. The results of this investigation can be used to develop optical elements for displays with vertical orientations of NLC molecules (MVA-display technology).

P.S.C.17.

**FEASIBILITY OF PRODUCING METAL OXIDE FILMS WITH TUNABLE
HIERARCHICAL POROSITY VIA ELECTROSTATIC SPRAY DEPOSITION**

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Metal oxide films with high pore volume and good pore connectivity enjoy a growing interest from fields such as catalysis, separation, sensing and power storage. A novel synthesis route to porous metal oxide films with controlled pore size was developed employing electrostatic spray deposition in combination with pore-templating. Pore size of titania coatings was adjusted by the choice of organic template co-deposited with the metal precursor (titanium(IV) isopropoxide). Employing amphiphilic block-copolymer Pluronic P123, PMMA latex spheres or a combination of the two, mesoporous, macroporous as well as hierarchically porous films were obtained in a simple and straight-forward manner. Direct control over layer thickness and total surface area of the coatings is achieved by extending deposition time as well as synthesis of multilayer coatings. The result prove the feasibility of producing metal oxide films with controlled hierarchical porosity via ESD.

P.S.C.18.

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

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We will demonstrate various applications of confocal Raman/fluorescence microscope integrated with Atomic Force Microscope (AFM) and SNOM to investigate modern nanostructures. First, we report on “classical” applications of such combination, when 2D AFM and confocal Raman maps are acquired simultaneously from the same part of the sample, but “independently” one from another. Physical characterization and modification capabilities of AFM merge with chemical resolution of confocal Raman microscope and general capabilities of optical microscope to provide complete information about sample investigated. Diffraction limited resolution of 2D Raman maps is 200 nm. We demonstrate results on various promising nanoelectronics materials: graphene flakes, carbon nanotubes, semiconductor nanowires etc.

The ultimate goal of integrating AFM with Raman/fluorescence spectroscopy is to break diffraction limit and to bring spatial resolution of optical methods down to resolution of AFM (a few nm). We present results of Tip Enhanced Raman Spectroscopy (TERS) mapping experiments 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). 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 resolution – determined not by the wavelength of light, but by the localization area of the surface plasmon electromagnetic field.

P.S.C.19.

**FEATURES OF POROUS BODY BASED ON HIGH MELTING TITANIUM
COMPOUNDS FORMED BY HIGH QUAZIHIDROSTATIC PRESSING
OF NANOPOWDERS**

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High quasihydrostatic pressures up to 5 GPa allows getting green body with density up to 85 % under conditions of intensive deformation even at room temperature. Thus, the green body has the homogeneously distributing porosity in the volume due to hydrostatic compression. The fixed level of compression stress provides the high-velocity densification of porous body, which lasts for 3 – 7 sec. Such a body containing defective deformed material can be effectively sintered without pressure.

The features of HP consolidation for TiN (80% mass) – TiB (20% mass) particulate composition in the field of static high pressures for up to 600 sec were analyzed. The sizes of coherent scattering field (CSF) changed in accordance with microdistortions of crystalline lattice ($\Delta a/a$) were studied in correlation with density of green body. These data were compared with that for the middle size particles of 30-40 micrometers previously obtained. The terms of compression providing full densification of the nanostructured green body during fixed exposure under invariable quasihydrostatic high pressure, were determined.

P.S.C.20

**SYNTHESIS AND CHARACTERIZATION Nb-TiO₂ SUPPORTED PLATINUM
NANOCATALYSTS FOR PEMFCs APPLICATIONS**

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Platinum based nanocatalysts at Nb-TiO₂ support were synthesized and tested as the catalysts for proton exchange membrane fuel cells (PEMFCs) applications. Nb doped TiO₂ catalyst supports, containing 0.5% and 5% of Nb, have been synthesized by modified acid-catalyzed sol-gel procedure in non-aqueous medium proposed by Boujday et al. BET and X-ray diffraction (XRD) techniques were applied for characterization of these supporting materials. Surface area and pore size distribution of the supports were determined from adsorption isotherms of nitrogen, applying gravimetric McBain method. XRD analysis revealed only a presence of anatase TiO₂ phase in synthesized support powder. Existence of any peaks belonging to Nb compounds has not been observed, indicating Nb incorporated into the lattice.

Nb-TiO₂ supported Pt nanocatalysts, were synthesized by borohydride reduction method. Synthesized nanocatalysts were characterized by TEM and HRTEM techniques applications. It was found homogenous platinum nanoparticles distribution over the Nb modified TiO₂ support with mean nanoparticle size of about 3 nm. HRTEM micrographs revealed no pronounced particle agglomeration.

Electrochemical techniques cyclic voltammetry and linear sweep voltammetry were applied in order to estimate catalytic activity of these new catalysts for both hydrogen oxidation and oxygen reduction reactions in acid solution. Nb(0.5%)-TiO₂/Pt exhibited better catalytic activity for both anodic and cathodic reaction. It was found ten times enhancement in specific catalytic activity (expressed in term of kinetic current density per real surface area) of Nb(0.5%)-TiO₂/Pt catalyst for oxygen reduction reaction in comparison with the carbon supported platinum (XC/Pt) nanocatalyst. Testing this catalyst for hydrogen oxidation reaction, small enhancement in catalytic activity was observed, comparing with the above mentioned XC/Pt catalyst. Having in mind that fuel cell performance is much more influenced by oxygen reduction reaction, owing its much higher overvoltage than hydrogen oxidation reaction, obtained results make this new catalyst promising for PEMFCs applications.

Keywords: Nb-TiO₂ support, Nb-TiO₂/Pt catalyst, Pt nanoparticles, PEMFCs.

P.S.C.21.

REFRACTION INDEX OF SUPERLATTICES

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In this paper, we have theoretically investigated some specific behavior of excitons in superlattices. Using the method of Green's function we have calculated dispersion law and the refractive index of these structures. It was determined that among wide variety of parameters which govern on calculus, only two parameters have a significant effect onto calculated energy spectra and optical values: a) the number of film layers which constitute superlattice; b) ratio of the exciton energy transfer between the layers of one film and on the boundary between two different films.

P.S.D.1.

**SYNTHESIS AND THERMAL PROPERTIES
OF NOVEL POLYURETHANE/CLAY NANOCOMPOSITES**

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Nanocomposites are inorganic/organic hybrid systems with matrix reinforced using nanosized particles. Layered silicates are the materials of choice for nanocomposite design because they exhibit very rich intercalation chemistry. Layered silicates may be chemically modified in order to be compatible with polymers for dispersion on a nanometer scale. In this work, polycarbonate-based polyurethanes hybrid materials were prepared by two different ways: one step technique and pre-polymerization procedure using tetrahydrofuran as a solvent. Hard domains of obtained materials consist of hexamethylene-diisocyanate and 1,4-butane diol chain extender. As soft segments of the network two polycarbonate diols (both of M_w ca 1000), differing in constitution of the polycarbonate chain, were used. The ratio of OH groups belonging to the diol and to the chain extender was kept constant ($R = 1$). Dibutyltin dilaurate was applied as a catalyst. All samples were reinforced by 1 wt. % of organically modified bentonite and montmorillonite nanoparticles. The main goal has been focused to determine the thermal properties of the materials obtained in the form of films and sheets. The glass transition temperature (T_g) of nanocomposites was estimated by modulated differential scanning calorimetry. In order to assess the service temperature range for possible applications, the thermal properties of the samples have been studied by simultaneous thermogravimetry and differential scanning calorimetry. It was found that T_g of the soft segments for all samples is about -32 °C. TG/DTG curves of the samples show that, up to about 300 °C, nanocomposites are chemically stable and the thermal stability is less influenced by their form. The addition of nanofillers stabilizes the structure of polyurethanes.

P.S.D.2.

**POLYMER-ORGANOCLAY HYBRIDS BY EMULSION POLYMERIZATION
INTO MONTMORILLONITE-VINYL MONOMER INTERLAYERS**

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Organic-inorganic hybrid materials with well-defined morphology and structure at the nanometric scale containing low amount (1–5 wt %) of chemically binded inorganic montmorillonite (MMT) nanofiller (Nanocor, Cloisite) were prepared by in-situ emulsion copolymerization. MMT particles were functionalized with quarternary ammonium salts containing polymerizable vinylic group and various length of alkyl chains. The organoclays have been employed as comonomers for copolymerization with butylmethacrylate, methylmethacrylate and styrene. The structure and physical properties of the prepared nanocomposites were studied by WAXS, SAXS, DSC, mechanical and dielectric spectroscopy. X-ray diffraction studies showed that all systems were swollen after monomer intercalation and the increase of interlayer d-spacing for monomer and polymer was dependent on the monomer composition.

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic (Project ME 09058).

P.S.D.3.

**THE EFFECT OF NON-BLACK FILLERS ON THE ACTIVATION ENERGY
AND MECHANICAL PROPERTIES OF EPDM VULCANIZATES**

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In this study the effect of two type non-black (NB) fillers: precipitated silica (SIL-1) and opalized white tuff (OWT) (primary particle size 9-16 μ m and 40 μ m) on activation energy and mechanical properties of ethylene propylene diene terpolymer (EPDM) rubber were investigated. NB fillers were added in range from 40 to 100 phr. Cure characteristics and mechanical properties of NB fillers reinforced vulcanizates were measured. The activation energy (Ea) from two high temperature rheokinetic curves ($T_1 = 180^\circ\text{C}$ and $T_2 = 190^\circ\text{C}$) were determined. The effect of both: type and content of NB filler on the mechanical properties before and after thermal aging was also investigated and the obtained data were interpreted. The values of mechanical properties such as tensile strength (TS), modulus at 200% and 300% elongation (M_{200} , M_{300}), elongation of break (E_b) and hardness depend of type and content of NB filler, were found.

P.S.D.4.

**SYNTHESIS AND THERMAL BEHAVIOR
OF MODIFIED UREA-FORMALDEHYDE RESINS**

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Urea-formaldehyde (UF) resins are the most widely used polycondensation resins today in manufacturing particleboards. They convince by their high reactivity and good performance in the production and by their low price. However, they lack in water resistance of the hardened resin owing to the reversibility of the amino ethylene bond and hence the susceptibility to hydrolysis. These needs can be overcome by introducing other components, such as, thiourea and thiosemicarbazide to the UF resin molecules. Mixes of inorganic nano-filler in a form of silicon dioxide with UF resins was studied with the aim to prepare for producing nontoxic chip boards. Polymer nano-composites consisted of polymer and inorganic nano-materials have good advantages in thermal properties. Nano-fillers have a modifying effect on the properties of UF resin. But the nano-fillers formerly used are all particles with sizes above micron grade, which have only small modifying effect. Nanoparticles with small diameters are surrounded by many atoms on the surface, which lack adjacent atoms and have dangling bonds and unsaturated properties. It easily combines with other atoms to become stable. Chemical activities of nanoparticles are excellent. Given this property, our test introduces nanometer silicon dioxide (nano-SiO₂), to be added to modified UF resin, which obtains favorable modifying results. The thermal stability of two modified UF resins with thiourea and thiosemicarbazide and nano-SiO₂ as a filler, was investigated by non-isothermal thermo-gravimetric analysis (TG), differential thermal gravimetry (DTG), differential thermal analysis (DTA) and differential scanning calorimetry (DSC) supported by data from IR spectroscopy.

P.S.D.5.

PROCESSING OF ALUMINIUM-BASED IN-SITU COMPOSITES USING HVOF SPRAYED NICKEL COATING

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The aluminium matrix composites were prepared by HVOF spraying of nickel powder onto the aluminium sheet's surface followed by annealing in a range of temperatures 600 – 630°C (solid state), 640 – 660°C (semi-solid state) and above 660°C (liquid state of aluminium). Layers containing the Al_3Ni_2 and Al_3Ni intermediate phase compositions were created at the interface between the original coating sprayed and aluminium matrix. Moreover nickel diffuse into the aluminium matrix and produce strengthening by stable Al_3Ni and metastable Al_9Ni_2 particles. The origin of continuous $Al_3Ni + Al$ eutectic band in aluminium matrix was observed at the temperatures higher than 650°C. The band thickness growth is dependent on a rate of aluminium liquid phase formation and can be fully controlled by dwell time on annealing temperature. The microstructures were obtained by light microscope (Olympus GX-51) and scanning electron microscopes (JEOL 840-A, Philips XL30). Chemical composition was estimated by energy dispersive microanalysis (EDAX). The layers and $Al + (Al_3Ni + Al_9Ni_2)$ band thickness measurements were realized by means of image analysis (NIS Elements AR).

P.S.D.6.

DETERMINATION OF RECYCLED AGGREGATE CONCRETE DEGRADATION BY RESONANCE FREQUENCY ANALYSIS

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The evaluation of the dynamic modulus of elasticity of twelve different concrete mix proportions as a function of the density, water absorption and degradations due to freeze/thaw cycles is presented in this paper. Pore system and saturation are the main factors for concrete frost resistance. The frequency analysis of ultrasonic waves in concrete after every 25 cycles was done. Dynamic modulus of elasticity was determination by resonance frequency analysis. This parameter is 35-50% smaller for concrete with recycled brick as aggregate than ordinary concrete. For all concrete mixes dynamic and static (measured by destructive testing) moduli of elasticity were compared.

Key words: dynamic modulus of elasticity, ultrasonic waves, frost resistance, recycled aggregate concrete

P.S.D.7.

**USE OF MAGNESIUM OXIDE-CEMENT BINDER IN COMPOSITES
BASED ON HEMP SHIVES**

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Hemp concrete is an insulation material made out of hemp shives with appropriate lime binder. It can be used in buildings, to cover masonry walls or to fill walls, floors or roofs in timber frame structure. In this paper are presented the results of experimental study of utilization MgO cement as calcium hydrate replacement in lightweight composites based on hemp shives with emphasis on determination of selected characteristics of hardened composites. The results of compressive strength and thermal conductivity show that MgO cement based on the milled caustic magnesite is suitable alternative in comparison to conventional binders used in hemp concrete. This material leads to new environmentally products as non-load bearing building materials.

P.S.D.8.

**THE VISCOELASTICITY OF ELASTOMERIC COMPOSITES BASED ON
POLYCHLOROPRENE RUBBER AND CHLOROSULFONATED POLYETHYLENE**

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The study of structure-property relationships for elastomeric nano-composites has acquired significance due to the broad range of applications as advanced materials. A detailed understanding of the general mechanism of rubber reinforcement is one key to develop new systems providing the performance enhancement needed. The incorporation of nano-particles to rubber compounds with subsequent conversion to a network by possible crosslinking method leads to a materials of great complexity. It is generally known that elastomers surface do not always exhibit desired resistance against chemical loads such as organic gases and solvents. Therefore, other approaches for improving the organic gas and solvent resistance of this materials are the use of rubber macromolecules which have a different polarity than the organic gas or solvent or the use of additives which affects the processability and elastomer final properties. To enhance the properties of reinforced elastomers based on more network precursors it is important to understand the material atomic-scale microstructure. Optimal reinforcing power can be achieved only if the filler particles are well dispersed in the rubber matrix. The goal of this applicative work was to study the viscoelasticity of composites based on rubber blend. Polychloroprene rubber (CR) and chlorosulfonated polyethylene (CSM) were used as network precursors. Precipitated silica and diatomaceous earth were used as reinforcing filler in the loading range from 0 to 35 phr. The crosslink density of the elastomers was determined by swelling measurement. Modulus and glass transition temperatures of composite samples were determined by dynamic-mechanical spectroscopy.

P.S.D.9.

**PROPERTIES OF THE SINTERED PRODUCT ON THE BASIS OF CLAYS
FROM THE MINE OF WHITE BAUXITE "BIJELE POLJANE"**

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The aim of this paper was to investigate the possibility to obtain the sintered product on the basis of clays from the mine of white bauxite „Bijele Poljane“, with satisfactory properties regarding volume shrinkage, fire resistance, total porosity and compression strength. The white bauxite deposits in the whole area of the mine „Bijele Poljane“ are characteristic for the presence of clay in the hanging wall and footwall. The geological composition of the deposit of white bauxite is very complex. The irregular alternation of different varieties of the content was manifested. This situation influences directly the possibility of usage and evaluation of this mineral raw material. White bauxites with less than 5% of the iron compounds content represent extraordinary raw material for the fire resistance industry. This type of bauxite represents the greatest part of the excavated resources. These bauxites, apart from oxides, aluminum hydroxides and iron, also contain clays. According to previous investigations they are kaolinite type clays with small amount of additives. In experimental section the characterisation of clays was performed (determination of chemical, mineral and granulometric content) as well as DTA and TGA analysis. The sintering process was done at the temperatures of 1000°C, 1100°C, 1200°C, 1300°C and 1400°C. The volume shrinkage during sintering, total porosity and compression strength were determined. The investigations in this paper should primarily give information about the possibility of evaluation of this clay type.

P.S.D.10.

**CALCULATIVE COLOUR ANALYSIS & PCA EVALUATION
OF OXIDATIVE PROCESS IN BASIL BASED PESTO SPREADS**

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Colour evaluation, by means of multivariate image analysis was applied on colour lightness changes, corresponding to enzymatic and non-enzymatic browning of mild-heat processed basil-based food emulsions. The colourgram of digitalized images, taken during oxidation of samples, was evaluated. Basic colour information was derived from frequency colour distribution for *RGB* (red, green and blue) and *HSV* (hue, saturation and value) colour system, while the Principal Component Analysis (PCA) was carried out by evaluating covariance matrix, for raw, mean centered and autoscaled matrix of the basic *R*, *G*, *B* colour information, and the evaluation of eigenvalues and eigenvectors for all three numeric models. Influence of metal-chelating protein lactoferrin and organic acids on changes in lightness frequency distribution (*L*), corresponding to browning, was determined.

The quantified SWOT (Strengths, Weaknesses, Opportunities and Threats) analytical method, presented also in this article, is the method of solving multi-variate problem. The data objects to be compared were pesto spreads on 0th and 30th day. The research of the main key factors (parameters of influence) took place in the evaluation, and also the collection of data represented by key factors. The weights of key factors are evaluated according to principal component analysis (PCA). The determined values of Peroxide Value (PV), Acid Value (AV) and OIT_{DSC} (for both 0th and 30th day) are the input values for SWOT calculation, while the weights are calculated. The used normalization method is made by using fuzzy set (0 – 1), and calculated as benefit-criteria normalization (the higher the better), or cost-criteria normalization (the lower the better).

P.S.D.11.

ATLAS OF MATERIALS STRUCTURES – AN USEFUL APPLICATION FOR STUDENTS IN THE FIELD OF MATERIALS SCIENCES AND ENGINEERING

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An application "Atlas of Materials Structures" is a freeware developed with the aim to extend subjects provided by Institute of Materials Sciences and Engineering to make them more attractive to students. The software is closely related with innovation of the IMSE subjects started two years ago. Within the application there are almost 60 materials prepared in detail (microstructures with individual phase description), used methodology (sample preparation, light and scanning electron microscopy) and also the testing interface, which can be used by teachers to create the tests for students in the software directly. Two fundamental materials groups are covered: (i) iron, steels and cast irons, and, (ii) nonferrous metals and their alloys. The current bilingual version of the application (English and Czech) can be used as a useful tool for the Materials Science subjects' education in English at the Universities across the Europe and United States of America. The application is available at: <http://ime.fme.vutbr.cz/Atlas/index.php>, the official websites of the IMSE, FME Brno UT.

P.S.D.12.

DESIGN OF "DSYHS FAMILY" USING "MAXSURF"

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"Maxsurf" is a 3D "key" program that is used for hull surfaces modeling. Hull design and modeling with Maxsurf is a very dynamic process. The large number of options and commands gave us the opportunity of creating various and complicated hull forms that would require months of work with the traditional methods. In this project the generation of DSYHS Family (Delf Systematic Yacht Hull) is chosen. The purpose of this work is developing a new experience in high speed ship design that has a major tourist impact.

Keyword : DSYHS, MAXSURF program, turist impact.

P.S.D.13.

HYDROSTATICS ANALYSIS FOR DSYHS FAMILY USING MAXSURF

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"Maxsurf" is a Software that is also used for Hydrostatics Analysis of DSYHS Family "Delf Systematic Yacht Hull Series" of the Model that has been designed above with : $L = 15.023\text{m}$, $B = 4.2\text{m}$, $T = 2.061\text{m}$, and its been imported in Hydromax. DSYHS Family takes into account the weather conditions giving the effects throw the simulation reaction.

The cases that we have discussed for our Model with $L = 15.023\text{m}$, $B = 4.2\text{m}$, $T = 2.061\text{m}$ are for Loading Conditions of 14ton, 15ton, 16ton with Heel Angle 30-90 degree. In all the cases our Model has result successful over a Sinusoidal Wave, over a Trohoidal Wave and in Still Water.

Keyword: DSYHS, Hydromax pro.

P.S.D.14.

ANALYSIS OF HARDNESS PROPERTIES FOR POLYPROPYLENE SPECIMENS WITH THE ADDITION OF GLASS POWDER

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This paper analyzes possibility of re-use of polypropylene through recycling with addition of glass powder, related to change of hardness. Standard specimens, made of polypropylene as a basic material and glass powder as an additional material, were examined together with secondary materials through six cycles of recycling. Specimen was made with the percentage of additional material of 5%, 10%, 15%, 20%, 25% and 30% of glass powder, with granulation less than 0,5mm. Basic hardness properties were also determined. The main goal was to show polymeric waste as a raw material, or as an exploitable material originated from partial separation of communal waste. Experimental data will give a possibility to form patterns of change in hardness properties of examined material, with addition of other material, through recycling cycles.

P.S.D.15.

FLY ASH INFLUENCE ON THE CHEMICAL AND MECHANICAL PROPERTIES OF CEMENT CONCRETE COVER OF PAVEMENT

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Recent production technologies in industries produce plenty of wastes that contain utilizable components and represents secondary raw materials. The fly ash utilization in concrete constructions for transport infrastructure leads to reduction of materials related problems. Additionally the documented research proved that the increase of the fly ash utilization provides a net of environmental benefits by reducing the landfill materials and the Portland cement demand. And last but not least it is the cost saved by the pavement building, where a lot of concrete mixture is produced and utilized.

The research of fly ash treatment for its use in building industry is oriented. The accent is given on its utilization in the Highway Engineers for the cement-concrete cover of pavement production. In cooperation with building praxis was tested the fly ash from brown (ENO Novaky) coal combustion. In accordance with the proposed recipe the specified amount of cement in fresh concrete mixture was replaced by 5-15 % ENO fly ash. Compressive strength and combined stresses strength after 7, 28 and 90 days of hardening composites as well as frost and chemical resistance were tested and compared with reference composite (the concrete C 30/37) which satisfies the requirements in accordance with the Technical standards.

P.S.D.16.

PROPAGATION OF GUIDED WAVES IN COMPOSITE STRUCTURE APPLICATION TO NON DESTRUCTIVE TESTING

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Fundamental to the understanding of guided wave analysis in NDT is the generation of phase velocity, group velocity dispersion curves. Dispersion curves are used to describe the relationship between frequency, phase velocity and group velocity, mode and thickness. In the case of a isotropic plate, the dispersion curves can be derived from the solution of the Rayleigh-Lamb equation. In the case of composite material it is not possible to find a close form solution of the dispersion curves because there are different methods (TM, GM, SM, etc.) that can be used to solve the problem. In this article we use the TM (transfer matrix) method applied to anisotropic laminated composite plates which is stable for low fd product values. We have solved dispersion curves for a layered plate A534/F252 of unidirectional fibers for different wave propagation orientations.

P.S.E.1.

**A PRELIMINARY STUDY ON THE DNA DAMAGE INDUCED
BY EXTRACTS OF UVAE URSI FOLIUM**

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The crude drug of *Arctostaphylos uva-ursi* (L) Sprengel (*Ericaceae*) known as *Uvae ursi folium* (UUF), also known as bearberry, contains three main groups of pharmaceutically relevant compounds: phenols, tannins and flavonoids, with arbutin (hydroquinone- β -D-monoglucopyranoside) being the main phenolic constituent. Water extracts of bearberry leaves, which contain high concentrations of arbutin, have been used in traditional medicine to treat urinary tract infections. Antibacterial activity is due to released hydroquinone from arbutin by the action of β -glucosidase. Methanol extracts of the drug have shown inhibiting effect on tyrosinase activity. This study was aimed at estimating the effectiveness of the water or methanol extract of UUF or coextract of UUF with almond meal (which contains high quantity of the enzyme almond β -glucosidase) to damage the DNA. The experiment was conducted at various time and extract concentration range against plasmid and calf thymus DNA. The results of an electrophoretic study showed that the methanol and water (co)extract induced the relaxation of supercoiled plasmid DNA to open circular and nicked linear forms of pUC18 plasmid. Additionally, the spectral changes in UV/Vis spectra of calf thymus DNA recorded in presence of the extracts were observed. The obtained results suggested that the water extract as well as methanol extracts of UUF showed higher damaging effects on DNA in the presence of crude extract of almond meal.

P.S.E.2.

**IN VITRO INTERACTION BETWEEN BONE MARROW CELLS
AND NANOMATERIALS CoHAp**

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Bone tissue reconstruction and reparation is big challenge in medicine. Biomaterials based on hidroxyapatite are widely used in reparation of bone defects. Bone marrow cells have great potential of differentiation in different cells of mesenhim tissue. The aim of this study was to investigate interaction between bone marrow cells growing in osteogenic medium with nanomaterials cobalt-substituted calcium hidroxyapatite nanopowders (CoHAp). In that purpose, powder nanomaterials CoHAp was dissolved in osteogenic medium to final concentration of 10 mg/ml, 1 mg/ml and 0.1 mg/ml. Bone marrow cells of Balb/c mice were seeded in tissue culture plates with different concentrations CoHAp. Cultures were grown for 2 week and were then evaluated by light and scanning electron microscopy Analysis showed that concentrations over 1 mg/ml nanomaterials CoHAp have cytotoxic effects on bone marrow cells in culture, while concentration of 0.1 mg/ml shows biocompatibility.

P.S.E.3.

**HISTOCHEMICAL OBSERVATION AND THE ANALYSIS OF BIOCHEMICAL
BONE REGENERATION MARKERS IN TREATMENT
OF AN OSTEOPOROTIC RAT BONE WITH Ca/Co-HAp NANOPARTICLES**

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One of the prerequisites for a good prosthetic rehabilitation is well preserved bone tissue. However, osteoporosis as a modern age disease often compromises a good dental treatment. Oral implantology offers a solution through the use of various biomaterials. Most researchers focus on the synthesis of the nanomaterials with magnetic and paramagnetic properties. The aim of this study is to examine the role of Ca / Co-HAp nanoparticles in the regeneration of the osteoporotic alveolar bone in experimental animals by analyzing the biochemical blood markers (ALP, Ca, Mg, and P) and through histochemical analysis. The research was carried out on female Westar rats, aged 6-8 weeks. The obtained results for the biochemical blood markers showed statistically significant rise. Histological analysis revealed high level reparatory skills of the biocomposite implanted in the bone defect as early as in the 6th week of the experiment as well as an increased alkaline phosphatase activity in the mineralized tissues. The implantation of the biomaterials facilitates osteogenesis, justifying their use in the accelerated regeneration treatment of the osteoporotic alveolar bone.

P.S.E.4.

TESTING THE ANTIMICROBIAL ACTIVITY OF HYDROXYAPATITE NANOPARTICLES IN VITRO

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Antimicrobial materials based on hydroxyapatite are very attractive for wide application in medicine and stomatology. The goal of this work was to test antimicrobial activity of hydroxyapatite nanoparticles Co/Ca- hydroxyapatite and biphasic calcium phosphate/ poly (lactide-co-glycolide) composite biomaterial. Antimicrobial activity of the samples was tested using dilution method and disk diffusion. The results of antimicrobial tests were obtained by determining the reduction percentage the number of bacteria in physiological solution where bacteria cells were exposed to the samples. It can be concluded that synthesized HAP biomaterials have satisfactory antimicrobial activity against tested bacteria strains.

P.S.E.5.

PGA CAPPED SILVER NANOPARTICLES FOR BIOMEDICAL APPLICATION

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Metallic nanoparticles possess unique electrical, optical and biological performances that have attracted considerable attention due to their potential use in many applications, such as catalysis, drug delivery, nanodevice fabrication, etc. Capped silver nanoparticles (AgNPs) have many biomedical applications due to its excellent biocompatibility, antiviral and antibacterial properties. However, in the literature it has been reported that bare silver nanoparticles can be toxic. This supports the idea that the toxicity is associated to the presence of bare metallic nanoparticle surfaces, while particles protected by the organic layer are much more biocompatible and thereby less toxic. Poly (α , γ , L-glutamic acid) (PGA) is a hydrophilic, biodegradable, and naturally available biopolymer. Its biological properties such as nontoxicity, biocompatibility, and nonimmunogenicity qualify it as an important biomaterial in drug delivery applications. In this study we used PGA as organic layer for silver nanoparticles. PGA capped silver nanoparticles were prepared by chemical reduction method with saccharides as reducing agent. The samples were characterized by particle analyzer, X-ray diffraction (XRD) and Ultraviolet Spectroscopy (UV).

P.S.E.6.

**IN VIVO AND IN VITRO INVESTIGATIONS OF IRON OXIDES NANOPOWDERS
INFLUENCES ON BLOOD**

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The influence of Fe-oxides nanoparticles obtained by electrochemical (EC) synthesis with and without (plane powders) organic surface layer cover on blood has been investigated, in vivo using Albino (Wistar) rats and in vitro, using 30 various donors human blood. The two characteristic magnetite powders obtained in EC cell at current density of 1000 mA/dm² and temperatures of T=20 °C and T=60 °C, and a ferro-fluid produced by use of citric acid have been used. Structure and morphology of the particles were investigated by X-ray diffraction (XRD), Scanning and Transition Electron Microscopy (SEM and TEM) and Z-titration techniques, magnetic properties using Faraday method and SQUID measurements, and specific electrical resistivity and infrared (IR) spectra have been also determined. Powder samples were introduced in rats as 0.5 ml 1:10 and 1:100 solutions, and changes of blood test, differential blood test and metabolic changes analysed after 24 hours using HmX-Coulter VCS (Volume-Conductivity-Light Scatter) apparatus. It has been established that ferro-fluid and plane powders influence blood in different ways, but that they are not harmful in any way in the used concentrations. Preliminary investigations of small power density (20 mW/cm²) laser light influences on human blood with and without magnetite nanoparticles dissolved have been conducted too.

P.S.E.7.

TOTAL PHENOLS AND ANTIOXIDANT ACTIVITY OF THE ACETONIC EXTRACT OF HALACSYA SENDTNERI

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The objective of this study was to investigate the total phenolic content and related antioxidant activity of the acetonic extract of *H. sendtneri*. The total amount of phenols, flavonoids and non-flavonoids was determined using Folin-Ciocalteu reagents, by a spectrophotometric method at 765 nm. The content of total phenols in the acetonic extract of *H. sendtneri* is 125.0 ± 5.01 mg GAE/g extract and that of flavonoids 64.63 ± 3.07 mg RU/g of extract (mean of three measurements). The antioxidant activity was determined using the DPPH free radical method. The reference standards used included ascorbic acid and BHT. IC₅₀ values were determined for all samples and amounted to 216.32, 5.99 and 12.77 µg/ml for the acetonic extract, ascorbic acid and BHT, respectively, for DPPH free radical activity. The results reveal the antioxidant activity of the acetonic extract and facilitate further research to identify antioxidant components.

P.S.E.8.

BIOREACTOR CHARACTERIZATION OF NOVEL ALGINATE NANOCOMPOSITES FOR BIOMEDICAL APPLICATIONS

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A biomimetic bioreactor with mechanical stimulation was utilized to evaluate novel alginate nanocomposites under *in vivo*-like conditions relevant for articular cartilage. Discs and/or packed beds of microbeads of alginate with or without Ag nanoparticles were tested at 10% strain in two regimes: at a loading rate of 337.5 µm/s and at sequential increments of 50 µm displacement every 30 min. Packed alginate microbeads exhibited up to 2-fold higher compression and equilibrium unconfined compression moduli than the discs, while the influence of Ag nanoparticles was negligible. In addition, alginate microbeads with or without immobilized cells were assessed under repeated cycles of dynamic compression in physiological regime (1 hr on/1 hr off, 0.42 Hz, 10% strain) for up to 15 days. These studies showed bioreactor potentials for estimation of biomaterial behaviour upon implantation.

P.S.E.9.

EROSIVE POTENTIAL OF SOME PHARMACEUTICAL PREPARATIONS ON ACRYLIC DENTURES

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In dental-prosthetic practice the most commonly used materials for total dentures production are acrylates. According to the basic chemical structure, these materials belong to methacrylate acid esters, usually methylmethacrylate. In order to improve the natural characteristics and achieving the right color of gums, certain inorganic substances such as grains of glass, zirconium silicates, aluminum oxides, salts of mercury, iron, cadmium and others are added to acrylic materials. Acrylic materials used for dentures production must have some level of biocompatibility. They should not be harmful to pulp cavity and soft tissue of the teeth, should not contain toxic substances and allergens and have cancerous potential.

Dentures in the oral cavity are exposed to the effects of saliva medium, food, beverages and remedial preparations of different flavors and temperature. Due to these influences, the dentures can be damaged and may result in the release of heavy metals, which may act toxic to human health.

In this study we followed the perservance of acrylic dentures exposed to citric acid and to the different pharmaceutical products, at different temperatures and at different times, by determining the content of lead and cadmium.

The content of these metals was determined by potentiometric stripping analysis (PSA) in the samples of new and used acrylic dentures made by cold and hot process of polymerization. The samples were treated with prepared solutions at temperatures of 4, 25, 37 and 50 °C for a period of 3 and 24 hours.

Analysis showed that sour taste pharmaceuticals have a corrosive effect on acrylic dentures, while the certain amount of lead was released, which varied depending on the method of production, time and temperature of exposure to these media. The highest content of Pb was released from acrylates made by cold process of polymerization. Highly toxic metal Cd was not detected.

P.S.E.10.

**NORMAL AND ABNORMAL APPEARANCE OF DIGESTIVE GLAND EPITHELIUM
SURFACE OF *PORCELLIO SCABER* STUDIED BY SEM**

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The aim of the investigation was to characterize structure of the digestive gland epithelium of a terrestrial isopod *Porcellio scaber*, using conventional scanning electron microscopy (SEM). The animals were collected at three unpolluted locations in Slovenia in order to provide evidence on morphology of the normal and abnormal gland epithelia. The samples of digestive system of animals were prepared for SEM by usual method of biological sample preparation. Morphological elements determined by SEM, were recorded and compared among animals such as the shape of the cells, presence and distribution of microvilli, presence of bacteria on the cell surface and extrusion of lipid droplets. In all investigated animals approximately 500 µm long regions was investigated in a detail and compared to some other regions in order to confirm the usual appearance of cells.

Keywords: Scanning electron microscopy. Digestive gland epithelium, Hepatopancreas, Isopoda, Crustacea

P.S.E.11.

**SWELLING, MECHANICAL AND ANTIMICROBIAL PROPERTIES OF
Ag/P(HEMA/IA)/PVP SEMI-INTERPENETRATING HYDROGEL NETWORKS**

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Recent trends have demonstrated that macroscopic gels are very promising as nanoreactors for *in situ* synthesis of nanoparticles, and this strategy has brought up a new concept in hybrid or composite systems in chemistry and engineering science. This methodology is noteworthy for the possibility to control the size and morphology of the nanoparticles by varying the amount of monomer, cross-linker, and functionality of gel networks. A few studies that deal with metal nanoparticles, especially silver, gold, and copper, have exhibited antimicrobial activity on microorganisms. Silver nanoparticles are considered because of nontoxic and environmentally friendly antibacterial materials, but due to their poor binding to surfaces, their utility is restricted. Therefore, embedding of polymer-stabilized nanoparticles in hydrogel networks is an outstanding approach for biomedical applications. In our study, we report the incorporation of silver nanoparticles in semi-interpenetrating hydrogel networks (semi IPNs) based on 2-hydroxyethyl methacrylate (HEMA) and itaconic acid (IA) networks, and poly(vinyl pyrrolidone) (PVP) as an interpenetrant. PVP was chosen due to its protection, reduction, and nucleation characteristics for metal nanoparticles. Silver/semi-IPNs samples were prepared through an optimized *in situ* solution crosslinking copolymerization of HEMA and IA, with ethylene glycol dimethacrylate (EGDMA) as a crosslinking agent, in the presence of PVP, a silver salt and a reducing agent. The samples were characterized by Fourier transform infrared spectroscopy (FTIR), dynamic mechanical analysis (DMA) and scanning electron microscopy (SEM). FTIR measurements confirmed the binding of silver nanoparticles into the polymer network. All samples showed good mechanical properties and a heterogeneous distribution of silver nanoparticles. Swelling and diffusion properties of silver/semi-IPNs were also measured. The equilibrium degrees of swelling values are in the range from 2.46 to 4.25. The values of the diffusion coefficient are from $(0.19 \text{ to } 4.48) \times 10^{-7} \text{ cm}^2/\text{s}$. Silver/semi-IPNs showed pH and temperature sensitive behaviour. Antimicrobial activity of samples was tested using *E. coli*, *S. aureus* and *C. albicans* strains. It turned out that antimicrobial performance depended on the hydrogel composition and the type of microbes. The smart silver/semi-IPNs reported here might be used as biomaterials for drug delivery devices, biosensors and in dermocosmetology applications.

P.S.E.12.

**NANO-RHEOLOGY OF POLYMER-CELL SYSTEMS IN THE COURSE
OF CELL IMMOBILIZATION**

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The entrapment of cells within hydrogel matrixes is a cell immobilization technique attractive for a variety of applications including food technology, pharmacy and biomedicine. Design of material and system structures is of basic interest for properties and performances of such cell-polymer "composites". Owing to the very gentle, simple and rapid procedure, the entrapment of cells in alginate hydrogels is still the most frequently used method for immobilization. It immediately provides efficient supply of cells by nutrients, good microenvironment conditions for cells inside the bead, decrease of cell leakage from beads, etc. However, much less explanation has been made on the micro- environmental restrictive effects in the course of further cell growth and development of cell colonies. A number of authors have reported early suppress of cell growth for different systems, but it is rather hard to describe more in detail the mechanism of that multi component and multilevel processes. Therefore, it is of considerable interest to establish rheological relations between cell and polymer matrix behavior in the course of development and grow of cell colonies inside hydrogel beads. Cell growth and movements produce local stresses in the polymer matrix and those nano –level changes can be related to the number of recent experiments with model systems investigating at nano –level both types of systems, i.e. cell movements or polymer matrix deformation. The integral approach can be formulated in terms of viscoelasticity of such composite systems. In this contribution the Zener-type constitutive equation is formulated for describing specific effects of energy dissipation due to interactions between cells with hydrogel parts and interactions between hydrogel parts themselves. Results indicate that for consideration of such complex phenomena constitutive equation with fractional derivatives are needed. The new relations for the long-time evolution of reversible part of stress within hydrogel are formulated and interpreted in terms of structural changes of the system.

P.S.E.13.

**EVALUATION OF VOLUME FUNCTIONS FOR FILLED HYDROGEL
NANO –STRUCTURES**

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The entrapment of particles within hydrogel matrixes is technique attractive for a variety of polymer applications including pharmacy, food technology and biomedicine. Of the basic interest for that is the choice of material and procedure of polymer matrix preparing. Owing to the very gentle, simple and rapid procedure, the confining of fine particles especially living cells in alginate hydrogel beads, is still the most frequently used method, in particular for cell immobilization for different biosystems. Significant attempts have been made to optimize the performances of such beads by ensuring appropriate conditions for their biotechnological functions. These functions depend on efficient supply of cells by nutrients, optimal microenvironment conditions for cells inside the bead, decrease of cell leakage from beads, etc. However, much less explanation has been made of the microenvironmental restrictive effects of cell growth. A number of authors have reported early suppress of cell cluster growth for different systems of immobilized cells in hydrogels, but it is rather hard to describe more in detail the mechanism of that multi -component and multi-level processes.

In this contribution is applied Jammed state thermodynamics for description of cell clusters in hydrogel. To elaborate more in detail cluster structure local differences at nano –level and cell-polymer local interactions as well, a number of Volume functions corresponding to Hamiltonians in Statistical mechanics of small systems has been formulated and integrated to compare with experimental results for alginate networks.

P.S.E.14.

**TEETH CHARACTERIZATION BY AFM/MFM
AND OPTO-MAGNETIC FINGERPRINT**

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In this paper we present the results of comparative investigation of magnetic properties of three main dental tissues: enamel, dentin, cement as well as caries of enamel, dentin and cement. The magnetic properties are examined by Magnetic Force Microscopy (MFM) and Opto-magnetic fingerprint (OMF). OMF is a novel method by which it is possible to derive the magnetic properties using an optical characterization method (based on interaction of light with valence electrons and coupled with digital image processing tools).

Bearing in mind that the orbital velocity of valence electron in atoms is about 10^6 m/s, this gives the ratio between magnetic force (F_M) and electrical force (F_E) of matter, of around $F_M/F_E \approx 10^{-4}$. Since force (F) is directly related to quantum action (Planck action, $h=F \times d \times t = 6.626 \times 10^{-34}$ Js, where F is force, d is displacement and t is time of action) this means that the action of magnetic forces is four orders of magnitude closer to quantum action than the electrical ones. Since quantum state of matter is primarily responsible for conformational changes on the molecular level, this means that detecting differences between tissue states is by far more likely to give greater sensitivity on the level of magnetic forces than it would be on the level of measurement of electrical forces.

Our results show that caries tissue is characterized with greater non-homogeneity in magnetism than healthy tissue, which can be observed from MFM and OMF image. This brings to attention two points: magnetic properties can be connected to health state of tissue and they can be detected rapidly and simply by OMF technique.

The perspective of applying this method to standard dental practice can be summarized in the following: enabling accurate objective early diagnosis of enamel demineralization (incipient decay) and enabling developments of preventive dental treatment methods.

P.S.E.15.

OPTICAL PROPERTIES OF NANOPHOTONIC CONTACT LENSES

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In this paper we present novel contact lenses materials composed of poly(methyl methacrylate-PMMA), and three types of nanomaterials (fullerene-C₆₀, hydroxlate fullerene C₆₀(OH)₂₄ and metformin hydroxlate fullerene C₆₀(OH)₁₂(OC₄N₅H₁₀)₁₂). Therefore, we investigated all three types contact lenses by UV-VIS spectroscopy, phase contrast atomic force microscopy (PC-AFM), magnetic force microscopy (MFM), and optomagnetic fingerprint (OMF) technique and found out that optical properties of nanophotonic lenses are more closer to human eye light sensitivity than classical contact lenses composed only of PMMA. Nanomaterials of contact lenses have influence on physical properties of light transmission and that these changes can be detected by UV/VIS spectroscopy as well as optomagnetism. These results carry significant biophysically based implications for contact lenses industry, biomedical application industry and applied optical science.

P.S.E.16.

CERVICAL SAMPLES ANALYSIS BY STANDARD PAPANICOLAU TEST AND NOVEL OPTO-MAGNETIC FINGERPRINT METHOD

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Cervical cancer and endometrial carcinoma are the most common invasive cancers of the female genital tract and account for 12% of all invasive cancer in women, excluding skin cancer and melanoma. In this study, we used 40 samples prepared for standard Pap test and examined them as double-blind experiment using digital imaging software that analyzes the difference between reflected diffuse white light and reflected polarized light (opto-magnetic fingerprint-OMF) in order to detect normal, dysplastic and cancerous cells. Samples were prepared, according to standard fixation and staining procedures used for Pap smear tests during regular colposcopic examination. To analyze opto-magnetic images of samples we used a digital camera customized for taking OMF pictures (DI-OMF) and light-mater interaction analysis software (DI-OMF), which guides the diagnostic decision to more refined distinction between normal smear and the one containing either dysplastic or cancerous cells. Since the application of OMF enables detection of significant differences between standard Pap test categories, especially in case of normal and pathological tissue states, this method offers an advantage over classical methods in the area of early detection of suspicious cells. To compare with standard Pap test, DI-OMF method has sensitivity 93.9% and specificity 87.5%. By this method it is possible to analyze the whole surface of the slide (smears) and obtain the result that is not dependent on the capability, subjectivity, experience and knowledge of the practitioner.

P.S.E.17.

**A COMPARISON OF BRACKET DEBONDING FORCES BETWEEN
THE TWO ADHESIVES: CON TEC LC AND CON TEC DUO**

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Fixed technique for applying brackets would be impossible without using adhesives for their fixation to the tooth enamel. However, the use of adhesives entails a number of problems which are a consequence of their imperfection, besides the fact that they have been actually applied for a number of decades already. The paper will analyse the debonding force values for bracket-tooth interface by using *Con Tec LC* and *Con Tec Duo*. For comparative analysis of the strength of bracket-tooth interface, with the application of different types of adhesives, 80 extracted teeth of the frontal region were used (central, lateral incisor teeth and canines of the upper and lower tooth arch). For the debonding process of applied orthodontics brackets, single-axial *Stretch system* for examination of tissues was used to determine the value of the force necessary to separate the bracket from tooth services, i.e. it was used to test the debonding force. The direction of the used force for debonding was under the angle of 90 degrees to the vertical axis of the tooth. By comparison of mean values of the strength of interface among the tested groups, it was determined that the highest average value of bond strength was with the group of teeth with which *Con Tec Duo* was used, a little lower mean value was recorded with the use of *Con Tec LC* adhesive. Based on the obtained results it is suggested that, if the tooth dislocation degree is larger, more pronounced which requires bigger activation of the arch, that is to say, a higher force for moving the tooth, it is necessary to use the adhesive with the strongest possible bracket-tooth bond, in order to avoid undesirable separation of the bracket from the tooth (*Con Tec Duo*), whereas if the degree of the tooth dislocation smaller, adhesives that realize weaker bracket-tooth bond can be used (*Con Tec LC*).

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Kruk, R.		22
Kübel, C.		140
Kulik, T.		7,18
Kuljanin-Jakovljević, J.		144
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