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General Scientific Meeting 2012

Abstract Book

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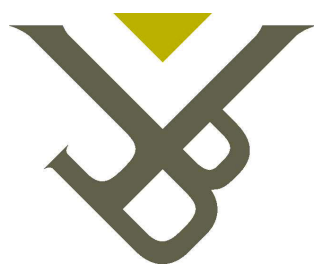
Vrije
Universiteit
Brussel

CONTENT

FOREWORD

Dear Participants,

Welcome to this Belgian Physical Society (BPS) general scientific meeting 2012 at the Vrije Universiteit Brussel. This year again, the BPS scientific meeting will propose three plenary talks by prestigious speakers. The first talk by A. Goobar on "Supernovae and the Accelerating Universe: the 2011 Nobel Prize in Physics" relates about the physics behind this year's Nobel Prize. With the second plenary talk, "MYRRHA: building a high power proton accelerator driven system for nuclear research and technology applications", P. Schuurmans presents the MYRRHA project by which Belgium takes a pioneering role in the field of reactor technology and related future developments. And last but not least, A. Barabasi will present his latest work on networks with his talk "Taming Complexity: From understanding to controlling networks".

Already several years now, the BPS organizes the young scientist contest with three finalists who will comptete in a special plenary contest session. On top of this, the best three posters will be given the European Physical Journal awards. The afternoon will be bustling with activities in the more specialized parallel sessions, for which the selection of topics and speakers is always a tremendously difficult task. We are convincend that the quality of all those presentations will reflect the research dynamism in Belgium.

We wish you a very good scientific day,

Gilles De Lentdecker, BPS President
Jacques Tempere, BPS Vice-President
Alexander Sevrin, President of the local organizing committee

PROGRAMME

08:30 – 09:00 Registration and coffee

09:00 – 09:15 Welcome by Gilles De Lentdecker, BPS President,
and Alexander Sevrin, President of the Local Organizing Committee

09:15 – 10:00 Plenary lecture 1
Ariel Goobar (University of Stockholm)
"Supernovae and the Accelerating Universe: the 2011 Nobel Prize in Physics"

10:00 – 10:45 Plenary lecture 2
Paul Schuurmans, (SCK-CEN, R&D Scientific advisor of the MYRRHA project)
"MYRRHA : building a high power proton accelerator driven system for nuclear research and technology applications"

10:45 – 11:15 Coffee, preview poster session, companies & institutes market

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11:15 – 12:15 Young Scientists Contest : oral presentations by the three finalists

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12:15 – 13:30 Lunch at the VUB Cafeteria

13:30 – 15:00 poster session, companies & institutes market
15:00 – 17:30 Parallel sessions
- Astrophysics, Geophysics & Plasma Physics
- Atoms, Molecules, Optics & Photonics
- Condensed Matter & Nanostructure Physics
- Fundamental Interactions & Nuclear Physics
- Biophysics and Medical Physics
- Physics and Education
- Statistical and Mathematical Physics

17:45 – 18:30 Plenary lecture 3
Albert-Laszlo Barabasi (Northeastern University, Boston)
"Taming Complexity: From understanding to controlling networks"

18:30 – 19:00 Closing ceremony : prizes and drink

PLENARY LECTURE 1

Auditorium QC, 9:15-10:00

Supernovae and the Accelerating Universe: the 2011 Nobel Prize in Physics

Ariel Goobar (University of Stockholm)

Observations of Type Ia supernovae over the last 2 decades have lead to a dramatic discovery about the expansion history of the Universe: instead of a slow-down due to gravitational attraction, the data indicates with very high significance that the expansion rate has been accelerating for about half the age of the Universe. This remarkable - and unexpected - result received the 2011 Nobel prize in Physics. The observational technique and challenges will be reviewed, along with a bit of history of how it has been to work in this field.

PLENARY LECTURE 2

Auditorium QC, 10:00-10:45

MYRRHA :
building a high power proton accelerator driven system for nuclear research and technology applications

Paul Schuurmans, , Hamid. Aït Abderrahim, Peter Baeten, Lucia Popescu, Rafaël. Fernandez
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Since about a decade SCK•CEN has been studying the coupling of a proton accelerator, a liquid Lead-Bismuth Eutectic (LBE) spallation target and a LBE cooled, sub-critical fast core. The project, called MYRRHA (**M**ulti-purpose h**Y**brid **R**esearch **R**eactor for **H**igh-tech **A**pplications), aims at constructing an Accelerator Driven System (ADS) at the SCK•CEN site in Mol (Belgium.

Presently, MYRRHA is conceived as a flexible fast spectrum irradiation facility, able to work as an ADS (subcritical mode) and as a critical reactor. MYRRHA will allow fuel development for new reactor systems, materials research for GEN IV and fusion reactors, radioisotope production and industrial applications, such as Si-doping. MYRRHA will also demonstrate the full ADS concept by coupling the accelerator, spallation target and subcritical reactor at a reasonable power level. This will allow the study of efficient transmutation of high-level nuclear waste and yield operation feedback, scalable to an industrial demonstrator.

The cooling of MYRRHA is based on the heavy liquid metal technology, using lead-bismuth eutectic. As a result, it will be able to contribute significantly to the development of Lead Fast Reactor Technology which is one of the key paths in Generation IV reactor development. In critical operation mode MYRRHA will be the European Technology Pilot Plant in the development roadmap for the Lead fast reactor.

MYRRHA is driven by high power proton accelerator with a beam energy of 600 MeV and a design beam current of 4 mA. Apart from the experimental and irradiation possibilities in the subcritical reactor, the MYRRHA proton accelerator on its own will be used as a supply of proton beams for a number of experiments. An interesting approach for fundamental research using the 600 MeV proton accelerator is the installation of an Isotope Separator On-Line facility (called *ISOL@MYRRHA*) with a ruggedized target-ion source system, which is able to provide intense low-energy Radioactive Ion Beams (RIB) for experiments requiring very long beam times up to several months. Experiments, requiring very high statistics, needing many time-consuming systematic measurements, hunting for very rare events, and/or having inherent limited detection efficiency, are particularly interested in extended beam times. This makes ISOL@MYRRHA complementary with the activities at other existing and future facilities. In a second phase, when the MYRRHA reactor will run as a stand-alone critical reactor, the full proton beam intensity could be used for ISOL@MYRRHA or other applications.

In March 2010, the Belgian federal government has committed itself to financing 40% of the total investment for MYRRHA. The remainder will be financed by an international consortium, that will be set up in the coming years. MYRRHA is foreseen to be in full operation by 2024.

This presentation will introduce MYRRHA, the status of the project and future plans.

PLENARY LECTURE 3

Auditorium QC, 17:15-18:30

Taming Complexity: From understanding to controlling networks

Albert-László Barabási[1,2,3]

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The ultimate proof of our understanding of biological or technological systems is reflected in our ability to control them. While control theory offers mathematical tools to steer engineered and natural systems towards a desired state, we lack a framework to control complex self-organized systems. Here we develop analytical tools to study the controllability of an arbitrary complex directed network, identifying the set of driver nodes whose time-dependent control can guide the system's entire dynamics. We apply these tools to several real networks, finding that the number of driver nodes is determined mainly by the network's degree distribution. We show that sparse inhomogeneous networks, which emerge in many real complex systems, are the most difficult to control, but dense and homogeneous networks can be controlled via a few driver nodes. Counterintuitively, we find that in both model and real systems the driver nodes tend to avoid the hubs.

YOUNG SCIENTISTS CONTEST

Auditorium QC, 11:15-12:15

11:15 – 11:35
YSC1   "The quest for polarized superfluidity: enhancing the FFLO state in a 3D Fermi gas"
Jeroen Devreese (Universiteit Antwerpen)

11:35 – 11:55
YSC2   "Dynamics of excitation waves in cardiac tissue"
Hans Dierickx (UGent)

11:55 – 12:15
YSC3   "Lattice location of transition metals in dilute magnetic semiconductors"
Lino Pereira (Katholieke Universiteit Leuven)

The quest for polarized superfluidity: enhancing the FFLO state in a 3D Fermi gas

Jeroen P.A. Devreese, Sergei Klimin, Michiel Wouters, and Jacques Tempere
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When a gas of atoms is cooled down to temperatures on the order of nanokelvin, new exciting phases and phenomena emerge. The primary example of this is the formation of a *Bose-Einstein condensate* (BEC) in a bosonic gas, in which a macroscopic fraction of the particles occupy the lowest quantum state. In a fermionic gas the situation is more complicated, since fermions are forbidden from occupying the same quantum state due to the Pauli principle, which hinders the formation of a BEC. However, a gas containing fermions in two different states (*spin-up* and *spin-down*) can circumvent this problem by forming *Cooper pairs* which consist of one spin-up and one spin-down fermion. These Cooper pairs behave as bosons and can condense into the *Bardeen-Cooper-Schrieffer* (BCS) superfluid state.

One of the questions that has attracted wide attention in the cold atom community is: what is the effect of *spin-polarization* (an unequal number of spin-up and spin-down particles) on the BCS superfluid state? Spin-polarization leads to spin-frustration: some particles will no longer find a pairing partner. This will hinder the BCS mechanism because less Cooper pairs can be formed.

So, what do experimentalists observe in a spin-polarized Fermi gas? Below a critical polarization, the BCS state can still exist, but only by cheating a little bit. Cheating in this case is called *phase-separation*: the BCS state expels the particles that cannot find a pairing partner. This trick does not work at higher polarization: in that case the system undergoes a transition to the normal state. The bottom line here is: the BCS state cannot accommodate spin-polarization.

So the question became: is there a superfluid state that <u>can</u> accommodate spin-polarization? Theoretically speaking, yes! In 1964, a candidate for polarized superfluidity was proposed which is called the *Fulde-Ferrell-Larkin-Ovchinnikov* (FFLO) state, named after its devisers. The difference between the BCS state and the FFLO state is that the former has Cooper pairs with zero momentum, while the latter has Cooper pairs with nonzero momentum. In contrast with BCS, it was predicted that the FFLO state can exist in a spin imbalanced system without needing phase separation. The problem is: this state has never been observed in experiment. This is in agreement with theoretical models, which predict that the FFLO state only occupies a very small sliver in the ground state phase diagram. Right now, many experimentalists are looking for this hitherto elusive state.

In this lecture, we present a new way to facilitate the search for FFLO. We show that adding a one-dimensional (1D) periodic potential to a three-dimensional Fermi gas results in a significant increase of the FFLO state in the ground state phase diagram. Starting from the free energy, calculated in the path-integral formalism, we construct the phase diagram of the system and study the FFLO stability region. Furthermore, the influence of the depth and the wavelength of the potential on the FFLO state is discussed. Finally we give a qualitative overview of the FFLO pairing mechanism under the influence of the 1D potential.

[1] **Jeroen P.A. Devreese, Sergei Klimin, and Jacques Tempere, Phys. Rev. A 83, 013606 (2011).**
[2] **Jeroen P.A. Devreese, Michiel Wouters, and Jacques Tempere, J. Phys. B: At. Mol. Opt. Phys. 44, 115302 (2011); Phys. Rev. A 84, 043623 (2011).**

Dynamics of excitation waves in cardiac tissue

Hans Dierckx, Henri Verschelde

(Ghent University)

Cardiac cells pass on electrical activity to each other, causing the cells to contract. Tachycardia is a persistent cardiac arrhythmia during which the electrical activity of the heart has the shape of a rotating spiral. When such spiral waves become unstable, a chaotic excitation pattern may arise, which is known as cardiac fibrillation. As the pumping function is entirely lost during fibrillation events, ventricular fibrillation is lethal within a few minutes. Unfortunately, the mechanisms that cause and sustain the states of tachycardia and fibrillation remain largely unknown.

In present-day cardiac modeling, the excitable properties of cardiac tissue are captured by a set of reaction-diffusion equations containing an anisotropic diffusion tensor D. We noted that the anisotropic diffusion term can be regarded as a covariant Laplacian, which enables to substitute local anisotropy for working in a curved space. Applying this curved space viewpoint, we successfully generalized findings from isotropic media, and extended the laws of motion for wave fronts and spiral wave centers to higher order. For example, we found that the local rotation of cardiac muscle fibers generates a negatively curved space, which slightly decreases the heart rate under tachycardia. Moreover, we noted that an increased rotation rate of cardiac fibers could cause tachycardia to decay immediately to ventricular fibrillation. This result may help explain why people with a particular cardiac geometry (e.g. sportsmen) are more susceptible to sudden cardiac death.

Lattice location of transition metals in dilute magnetic semiconductors

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The discovery of a dilute magnetic semiconductor (DMS) which is ferromagnetic above room temperature is a critical step towards the development of semiconductor spintronics [1]. For a given impurity-host combination, the magnetic behavior is largely determined by the lattice sites occupied by the magnetic impurities. The canonical example is Mn-doped GaAs (narrow-gap), where Ga-*substitutional* Mn orders ferromagnetically and *interstitial* Mn acts as a compensating defect which reduces the Curie (ordering) temperature. The situation is somewhat different in wide-gap DMS materials such as Co- and Mn-doped ZnO and GaN, for which it is generally accepted that the transition metals occupy only cation substitutional sites.

We present electron emission channeling experiments on the lattice location of implanted Mn and Co in GaAs [2], ZnO [3] and GaN. The technique is based on *channeling* and *blocking* effects acting on the β^- particles emitted during decay of radioactive ^{56}Mn and ^{61}Co impurities implanted at the ISOLDE facility at CERN.

In Mn-implanted GaAs, we show that while the majority of the implanted Mn impurities occupy substitutional Ga sites, up to ~30% occupy tetrahedral interstitial sites with As nearest neighbors. Contrary to the general belief that interstitial Mn is removed by thermal annealing at ~200ºC [4,5], we show that the interstitial fraction persists above 400ºC [2]. We discuss the implications of such high thermal stability of interstitial Mn on the strategies and prospects for achieving higher Curie temperatures in Mn-doped GaAs.

In Co- and Mn-implanted ZnO [3] and GaN, in addition to the expected majority in cation sites, significant fractions (~20%) of the implanted Co and Mn impurities substitute the anion (O in ZnO and N in GaN). We compare these results to previous lattice location studies on ZnO and GaN and discuss how such minority anion-substitution, which had never been considered before, may in fact play an important role in determining the materials' magnetic behavior.

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[3] L. M. C. Pereira, U. Wahl, S. Decoster, J. G. Correia, L. M. Amorim, M. R. da Silva, J. P. Araújo, and A. Vantomme, *Phys. Rev. B* **84** (2011) 125204.
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BEST POSTER CONTEST

13

The prizes for the three best posters are awarded by EPJ

BP1 [D9]

Characterization of BEGe detectors in the HADES underground laboratory in view of their application to neutrinoless double beta decay searches

Erica Andreotti[1] for the GERDA collaboration

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A complete characterization of newly produced Broad Energy Germanium detectors (BEGe), enriched in the isotope ^{76}Ge, is being carried out in the HADES underground laboratory, located 225 m below ground in Mol (Belgium). These detectors have been produced in the context of the GERDA experiment, searching for the neutrinoless double beta decay of ^{76}Ge. An important feature of BEGe detectors is their enhanced pulse shape discrimination, which allows in particular discriminating neutrinoless double beta decay from gamma-ray background events.

The aim of the characterization consists in the determination of all the important operational parameters of such detectors, like the active volume, the dead layer thickness and uniformity over the surface and to test the performance of the diodes in terms of energy resolution and quality of pulse shape discrimination.

The tests are being performed in the HADES underground laboratory in order to minimize the germanium exposure to cosmic radiation and the consequent activation, which could otherwise increase the intrinsic background of the detectors. The sand-clay overburden of about 500 m water equivalent assures in fact a muon flux reduction factor of about 5000 [1]. Two types of mechanical set-ups have been designed for the tests and deployed to the HADES underground laboratory, where a dedicated area has been allocated. One type consists of a simple measurement table, with a lead shield surrounding the detector, suitable for measurements with a test source placed in fixed positions (collimated or uncollimated). A second one is provided with a movable, motor controlled arm, which allows performing an automatized full area scanning of the diode with a collimated source. The latter is particularly suited for determining the dead layer thickness and uniformity of the whole surface, in order to detect any potential charge collection deficiency. Automatized acquisition systems, both analog (MCA) and digital (FADC), will be run in parallel in order to fully exploit the features of both systems.

This work aims at describing the characterization procedure and the measurement setups, as well as the preliminary results obtained and the potential applications which can be derived.

References

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BP2

GRBs and AGN researches in IceCube

Lionel Brayeur, Martin Casier and Ben Dumoulin

Vrije Universiteit Brussel – IIHE (ULB-VUB)

The Universe is full of not yet or not fully understood processes. Among all these phenomena, the Gamma-Ray Bursts (GRBs) and the Active Galactic Nuclei (AGN) are one of the most violent and energetic events in our Universe. Furthermore, the GRBs are the most luminous ($L \sim 1050$ erg s-1) ones. GRBs and AGN are the most potential candidates for the sources of the ultra-high-energy cosmic rays (1015-1020 eV).

Physicists have devised several models to explain the non-thermal processes that are taking place inside these objects. According to hadronic models photons are produced by the proton collision with photons present in the jet. These collisions produce neutral and charged pions which decay producing very high energy gamma-rays and neutrinos. Detection (or no detection) of these neutrinos therefore remains crucial for the under- standing of GRBs and AGN.

The IceCube Neutrino Observatory, located at the geographic south pole, has been designed to detect astrophysical neutrinos and represents thus a real opportunity to detect the GRBs' and AGN's neutrinos.
The present status of GRB and AGN analysis with IceCube will be presented in this poster.

BP3

Ultracold gases as a quantum simulator for the polaron

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In recent years ultracold quantum gasses have revealed themselves as quantum simulators for many-body theories and in particular for those developed in the context of condensed matter physics. An example of such a system is an impurity in a Bose-Einstein condensate: this can be mapped onto the polaron which describes the quasiparticle consisting of an electron interacting with lattice vibrations. The polaron Hamiltonian has not been diagonalized analytically making it the subject of many approximation schemes of which the Jensen-Feyman variational path integral is the most general. In the weak polaronic coupling regime this approximation was experimentally confirmed to be very accurate. A comparison of the optical absorption in the strong polaronic coupling regime with diagrammatic Monte-Carlo calculations on the other hand leads to discrepancies. These have not been resolved experimentally since there is no known material that exhibits this regime.

We present a polaronic treatment based on the Jensen-Feynman variational path integral of an impurity in a condensate. This allows us to calculate the ground state properties and the response to Bragg scattering [1,2]. All typical polaronic features are retrieved and it is shown that an experimental realization is realistic. Furthermore the use of a Feshbach resonance allows a tuning of the polaronic coupling strength. This suggests it is possible to probe the polaronic strong coupling regime for the first time with this sytem. A comparison of our results with an experiment and with diagrammatic Monte Carlo calculations will shed light on important unresolved questions regarding the polaronic strong coupling regime.

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BP4

Supernova Neutrino Detection with IceCube

D. Heereman von Zuydtwyck

Vrije Universiteit Brussel – IIHE (ULB-VUB)

The IceCube Neutrino Observatory, situated at the geographic South Pole, was completed in December 2010. A lattice of 5160 photomultiplier tubes monitors one cubic kilometer of deep Antarctic ice in
order to detect neutrinos via particle induced photons. The topic of this presentation is IceCube's response to MeV neutrinos generated by core-collapse supernova explosions of nearby massive stars.
This unique telescope was designed to detect energies greater than 100 GeV. Due to subfreezing ice temperatures, the photomultipliers dark noise rates are particularly low. Therefore IceCube can also
detect large numbers of MeV neutrinos by observing a collective rise in all photomultiplier rates on top of the dark noise. In the case of a supernova at the galactic center, IceCube's sensitivity matches that of
a background free megaton-scale supernova search experiment and decreases to 20 and 6 standard deviations for star explosions at the galactic edge (30 kpc) and the Large Magellanic Cloud (50 kpc),
respectively. IceCube's sensitivity of measuring several neutrino properties such as the neutrino hierarchy is addressed. Interesting signatures and characteristics of such a star explosion, i.e. the neutronization burst, the shock wave itself or the formation of its successor being a quark star or a black hole, will be investigated in order to demonstrate IceCube's detection capability for supernovae.

BP5 [D8]

Muon Counting study using IceTop

Haj Ismail

Universiteit of Ghent

Construction of IceCube, a cubic kilometer neutrino detector, was completed at the end of 2010. It consists of 5160 digital optical modules (DOMs) distributed over 86 strings buried between 1450 and 2450m deep in the Antarctic ice at the South Pole. The surface component of IceCube is the extensive air shower array, IceTop. IceTop consists of 81 stations over 1km^2 area. Each station has two cylindrical tanks placed 10m from each other and filled with ice. Each tank contains two DOMs to detect the Cherenkov radiation emitted by charged particles created in the ice.

IceTop is used to study charged cosmic rays with energies between 100TeV and 1EeV. Cosmic ray air showers are dominated by electrons and muons at the ground level. In this poster we will show an overview of the method we use to extract the muon contribution from the total signal created by all particles in the shower and use it to study the chemical composition of cosmic rays.

BP6 [C10]

Characterization and superconducting properties of a superconductor/ferromagnet hybrid system with Co clusters embedded in a Sn matrix

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The superconducting properties of hybrid systems consisting of ferromagnetic clusters randomly distributed in a superconducting Sn matrix were studied. Preformed Co clusters with typical diameters around 2 nm are produced with a laser-vaporization cluster source and have been co- deposited with thermally evaporated Sn on liquid nitrogen cooled SiO2-substrates. Structural characterization of the samples has been done by means of atomic force microscopy and Rutherford backscattering spectrometry. The magnetic and superconducting behaviour of these systems was studied by SQUID magnetometry measurements.

The magnetic behaviour of the Co clusters varies from superparamagnetic to ferromagnetic with increasing amount of embedded Co clusters. The superconducting critical temperature and phase boundary are investigated for different concentrations of Co clusters, ranging from 0 to 30 volume percent.

For the lowest concentration of Co below 20 volume percent, the Co clusters are superparamagnetic. Above 100K, reversible magnetization curves are observed. For higher concentrations of Co, the Co clusters interact with each other and behave as ferromagnetic particles up to 300K. In both regimes, the hybrid systems show superconducting behaviour with a clear increase of the steepness of the phase boundary. For the lowest concentrations of Co, no significant change in TC is observed. The highest concentration of Co did show a decrease of the superconducting critical temperature.

BP7 [D7]

Phenomenology of Scalar Top Pair-Production at the LHC

Thomas in't Veld*

Master student KULeuven PHENO group VUB

Phenomenology of beyond-the-Standard-Model physics is a rapidly evolving domain due to the enormous amounts of data being collected by, among others, the Large Hadron Collider. In the past decade, various tools have been developed to simulate and test the various theoretical models in an experimental context; with tools like MadGraph/MadEvent1 and FeynRules2. we now have a very efficiënt way to complete the chain from theoretical to experimental particle physics.

Supersymmetry is still one of the more satisfying symmetries to extend the Standard Model with. Although the parameterspace for viable supersymmetric extensions of the Standard Model has been ever shrinking with increasing data from collider experiments, there are still very good reasons to investigate SUSY models (like for instance the hierarchy problem for the Higgs boson mass, dark matter candidates, and the uni cation of coupling constants at high energies).

Various models of supersymmetry breaking induce different mass spectra of superparticles; where in most sce- narios the neutralino is the lightest supersymmetric particle (or LSP) and the superpartner of the top quark (the scalar top or stop) is the next-to-lightest susy particle (or NLSP). We investigate scenarios for different masses of the stop and the neutralino, and study hadron collision processes where a pair of scalar tops is produced - with the stops subsequently decaying to neutralinos and Standard Model top quarks.

We will discuss relevant experimental observables to differentiate a supersymmetric scalar top pair-production from the standard model background (pair-production of top quarks).

BP8 [B7]

Saturated green phosphors for LED applications

Jonas Joos, Katrien W. Meert, Anthony B. Parmentier, Jonas Botterman, Dirk Poelman, Philippe F. Smet

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Solid state light sources possess several advantages over traditional light sources (like incandescent or fluorescent lamps), including a long lifetime, high efficiency, small footprint and the absence of toxic substances. While for general lighting applications a wide emission spectrum is preferred to increase the colour rendering, display applications require light sources with a saturated emission colour [1]. In this work, we explore green luminescent materials which can efficiently convert the emission from a blue light emitting diode (LED). First a variety of phosphors hosts (including $SrSi_2O_2N_2$, $Ba_3Si_6O_{12}N_2$, $ZnGa_2S_4$ and $SrGa_2S_4$) are doped with divalent europium, and evaluated in terms of luminescence properties, thermal quenching and efficiency.

Then $Sr_{1-x}Eu_xGa_2S_4$ phosphors are studied in more detail over a wide dopant concentration range (x = 0.01 to 0.3), as function of temperature. The phosphors show a saturated green emission, with a peak wavelength around 536nm and a FWHM of 50nm. The internal quantum efficiency is 71% for x = 0.04. For this concentration, the emission intensity at 400K is still 90% of the intensity at room temperature. By measuring decay and thermal quenching profiles as a function of europium concentration, we were able to explain the emission properties on the basis of the local environment of the europium ions in the lattice [2].

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BP9 [C6]

Two-band superconductors: Hidden criticality deep in the superconducting state

L. Komendová, Y. Chen, A. A. Shanenko, M. V. Milošević, F. M. Peeters

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We found that two-band superconductors harbor hidden criticality deep in the superconducting state, stemming from the critical temperature of the weaker band taken as an independent system [1]. For sufficiently small interband coupling the coherence length of the weaker band exhibits a remarkable deviation from the conventional monotonous increase with temperature, having a pronounced peak close to the hidden critical point. This can strongly affect most of the superconducting properties, and can be experimentally observed (in e.g. multigap borides and pnictides) by imaging of the variations of the vortex core in a broader temperature range. In particular the effects crucially depending on the disparity of the characteristic length scales (e.g. nonmonotonic intervortex interaction [2], appearance of fractional vortices in mesoscopic samples [3]) shall be most pronounced in the vicinity of this hidden criticality.
We will present the analytic proof that the interband coupling is the governing field of this criticality with the same critical exponents as e.g. the magnetic field in the ferromagnetic materials. Furthermore, we will show the numerical results for the evolution of a vortex core with temperature obtained in the microscopic Bogoliubov-de Gennes formalism, which not only proves the existence of hidden criticality, but also motivates further experiments on multiband materials.

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2. E. Babaev and M. Speight, Phys. Rev. B 72, 180502(R) (2005).
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BP10

**Searching for neutrinos from Dark Matter annihilation in the Earth
with the IceCube detector**

Jan Kunnen

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Many models predict that heavy celestial bodies capture dark matter, and that these particles will self-annihilate. These annihilations may produce standard model particles, including neutrinos.

Large scale neutrino telescopes, such as the cubic kilometre IceCube Neutrino Observatory located at the South Pole, can be used to search for such neutrino fluxes. One of the celestial sources of interest is the Earth. Recent calculations indicate that the dark matter annihilation rate in the centre of the Earth, and thus the resulting neutrino flux , could be greater than that initially predicted for low mass (<100 GeV) WIMPs, and within reach of a large neutrino detector.

The status of the first search for Earth WIMPs with the IceCube detector will be presented.

BP11 [C22]

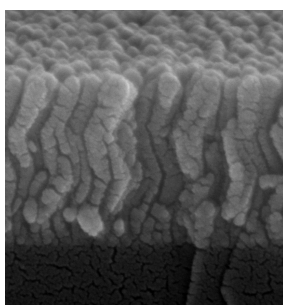**Nanostructured thin films for Solid Oxide Fuel Cells: crystallographic properties**

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Ghent, Belgium

A fuel cell converts the chemical energy from a fuel into electricity through a chemical reaction. The fuel is oxidized at the anode, while oxygen reacts on the cathode. The cathode and anode are separated by an electrolyte. In Solid Oxide Fuel Cells (SOFC) the electrolyte is an oxygen ion conductor such as Yttria Stabilized Zirconia (YSZ). To lower the process temperature of the SOFC the film thickness of the electrolyte must be reduced. The bulk properties of these materials are well known but when down scaled to a thin film the fundamental aspects of the oxygen ion conduction change due to the occurrence of small scale or nano-effects. That is why, a good understanding of the microstructure and crystallinity would open the possibility to manipulate the ionic conductivity by controlling the nanocrystalline microstructure of the thin film.

With dual magnetron sputter deposition, thin films of solid state electrolytes can be grown. This technique allows the deposition of thin films ranging in thickness from a few nanometers to micrometers and to investigate the compositional influence in a flexible way.

In this study the experimental conditions were varied to modify the microstructure and texture of the YSZ thin films. Especially the pressure, and the source-substrate distance showed an interesting influence on the thin film properties. From crystallographic point of view the films show the interesting feature of biaxial alignment. The crystals have a preferential out-of-plane and in-plane alignment, meaning that for a low misorientation angle, between the adjacent grains, the crystallographic properties of the polycrystalline thin film are comparable to a single crystal thin film. The films are built from well-defined V-shaped facetted columns. The constituent columns are tilted towards the zirconium source. This behavior has been investigated in more detail, and can be tuned by changing the geometrical configuration of the deposition set-up. As a result, zig-zag nanostructured columns can be grown.

BP12

Light backscattering in plasmonic films for enhanced gas and vapour sensing

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Based on recent experimental and theoretical results obtained with gold-glass nanocomposite films, we propose a plasmonic device which uses the backscattering of light in order to make a highly sensitive gas/vapour sensor. The backscattered reflectance is used as sensing signal since it has been shown that this component of the diffracted light is much more sensitive to a change of refractive index in the surrounding medium than the specular component. In addition, the backscattering of light presents an azimuthal angular dependency which is viewed as an advantage for practical implementation.

The device consists of three planar layers. First, a glass substrate acting as incidence medium. Then a layer with a reduced refractive index with respect to the substrate is added. This layer acts as a leaky-waveguide in order to maximize light coupling into the third sensing layer. The third layer is composed of gold nanopillars embedded in a SiO_2 matrix. Through numerical simulations, 2D periodic square and hexagonal arrays of gold nanopillars are compared in order to point out the influence of the nanocomposite arrangement in the photonic response. Moreover, disorder is introduced into these arrays in order to highlight the robustness of the sensing principle with respect to defects in the particlearrangement and size. For the purpose of gas/vapour sensing, we study the backscattered reflectance as it changes according to modifications in the dielectric environment at the external surface due to adsorption from gas/vapour. We determine the optimized device parameters and incidence angles.

Keywords: plasmonic device, backscattering of light, nanocomposite films, gas and vapour sensing

BP13

Theoretical investigation of the ionization and electronic dynamics induced by short pulses in ABCU

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Recent advances in the synthesis of ultra-short laser pulses have paved the way for controlling and probing of the electron dynamics[1]. With the aim to describe attosecond pump probe experiments, we investigated theoretically the electronic dynamics induced by short pulses as well as the effect of intense static electric fields on the ionization rates of molecules. An attosecond pulse can be used as pump to build an oscillatory, non-stationary, electronic state that exhibits localization of the electron density in different parts of the molecule both during and after the pulse. We used a time dependent multiconfigurational approach to describe the electronic dynamics induced by short pulses on the medium size molecule, ABCU (fig. 1). The coupling between the electronic states induced by the strong pulse is included in the many electron Hamiltonian used to compute the electron dynamics. We show that it is possible to implement control of the electron density stereodynamics (Fig. 2) in this medium size molecule by varying the characteristics of the laser pulse[2], for example by polarizing the electric field either along the N-C axis of the cage, or in the plane perpendicular to it. Due to the high intensity of the short pulses used to excite the system, ionization can occur. We investigated the effect of ionization by strong static fields using an effective Hamiltonian technique[3] based on the Feshbach partitioning of the space into bound and continuum states. We computed the ionization widths of the ground and excited states of the ABCU molecule as a function of the total energy of the system. We also computed the dependence of the photoionization spectra with respect to the strength of the static electric field in order to obtain information about the stability of the system in strong field.
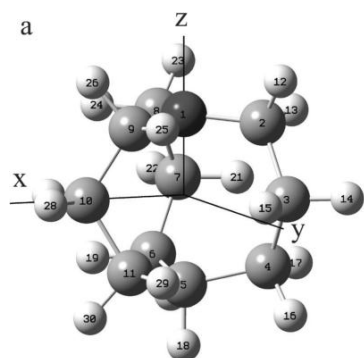
Fig. 1 Equilibrium geometry of ABCU ($NC_{10}H_{19}$) computed at the CAS(8,13)/6-31++G(d,p) level.
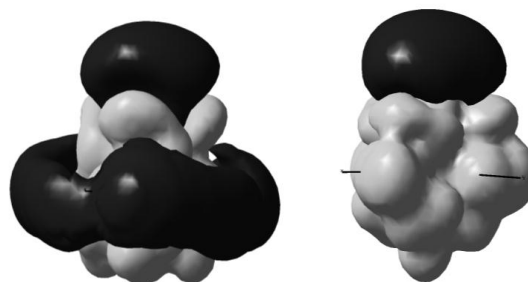
Fig. 2 Isocontour of the density difference between the density at time t=0 and t=14.4fs (left) and t=14.9 (right) induced by a short pulse polarized along z. The dark part represents the accumulation of electronic density.

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High sensitivity of the optical response of porous natural photonic structures to the presence of gases and vapours

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Structurally coloured natural photonic crystals (found in butterflies, beetles and other insects) are made of ordered porous chitin structures. In such photonic crystals, colour changes can be induced by relative gas/vapour concentration variations in a mixed atmosphere. For instance, when the composition of the atmosphere changes, the colour of Morpho sulkowskyi butterfly is modified [1]. Based on this effect, Potyrailo and coworkers demonstrated experimentally the possibility to identify closely related vapours [1]. They explained their observations by the occurrence of different spatial periodicities in the nanostructures from different regions of the butterfly wing: different photonic crystal periods are thought to be responsible for the wavelength selective optical response [1]. Recently, Biró and coworkers investigated four butterfly species and demonstrated fast, reproducible species-dependent selective sensitivity to seven test vapours [2].

In spite of increasing interests for such sensors, the fundamental mechanisms at the origin of the selective optical response are still not well understood.

The point is that refractive index variations resulting from the introduction of a specific gas species in the atmosphere are too small to justify entirely the dramatic changes observed in the optical response. Here, we demonstrate through numerical simulations that indeed gas/vapour-induced refractive index changes (typically $\Delta n \approx 10^{-6} - 10^{-7}$ between dry air and 50% relative humidity water vapour) are too small to produce a significant modification of the spectral reflectance in a representative 3D periodic model of natural porous nanostructures. For this purpose, we used a rigorous coupled wave analysis method for modelling light scattering from inhomogeneous optical media. The origin of the reported colour changes has therefore to be found in chemical modifications of the porous material and their impact on the photonic response.

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[2] Biró L. et al., Proc. SPIE, 2008.

BP15 [C13]

Superconducting proximity effect with Pb nanoparticles embedded in an Al matrix

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We investigate the superconducting properties of Pb nanoparticles (with a diameter varying between 8 and 20 nm) synthesized by ion implantation and subsequent annealing in an Al matrix. The critical temperature T_c of those new types of superconductors is found to increase linearly with the Pb/Al volume ratio. The experimental data is in excellent agreement with the theoretical predictions of the proximity effect in the Cooper limit for strongly coupled superconductors. The remarkably good agreement between theory and experiment implies that the quality of the interface between the nanoparticles and the Al matrix is very good (high transparency). Furthermore, the critical fields and critical currents of those hybrid superconductors have characterized extensively to obtain their full phase diagrams and analyze in detail their physical properties.

BP16 [C16]

Changing magnetic properties of nanocluster assembled films using hydrogen

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Using preformed gas phase Co nanoclusters and subsequent deposition thin nanogranular films were produced. These films were characterized using magnetic force microscopy and vibrating sample magnetometry. Tailoring of the magnetic properties in these nanocluster assembled films was achieved by admitting a small percentage of H_2 gas (~2%) into the Co gas phase formation chamber prior to deposition. The oxygen content in the films is considerably reduced by the presence of hydrogen during the cluster formation [1], leading to enhancement of magnetic interactions between clusters. This hydrogen-passivation method can be used to tailor the oxidation level thus controlling the magnetic properties of ferromagnetic cluster-assembled films. Further a method was tested to estimate the exchange field and the exchange constant in the samples. This model is originating from the random anisotropy model. For nanocluster assembled thin films an experimental formula for 3 dimensions was taken from reference [2]. Our results are in agreement with this experimental formulation in the case of the sample produced with H_2 gas.

References
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BP17

Phase-space dynamics of 2D topological insulators

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In the realm of Ehrenfestís theorem, classical trajectories obeying Newtonís laws have been proven useful to construct explicit solutions to the time-dependent WignerñLiouville equation[1][2]. By properly incorporating the e§ects of an applied magnetic Öeld and possible geometric constraints on the particles motion, we were able to Önd a solution for the integer quantum Hall e§ect in terms of classical phase-space trajectories. In view of this result and the recent interest in so called topological insulators we will show that systems with strong spin orbit interaction can also be described by this method if one deÖnes a four-component Wigner function. Under speciÖc conditions the equation of motion becomes a Klein-Gordon equation for either massive or massless particles. Following Bernevig et. al.[3], we show that this state can be realized in mercury tellurideñcadmium telluride semiconductor quantum wells .

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BP18

First-principles investigation of titanium and titanium dioxide adsorption on graphene

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Graphene with its uncommon electronic properties provides an open playground for chemical modification of its surface. The study of adsorption of metals and insulators is essential for further application in electronic device construction and to understand the impact of electrical contacts on the electronic properties of graphene.

We have performed ab initio ground state calculations for titanium and titanium dioxide decorated graphene. This includes the investigation of adsorption of a single titanium and titanium dioxide molecule, a covalently bonded titanium monolayer also as a weakly physisorbed monolayer of titanium dioxide crystal. Ground state structures were calculated with corresponding binding energies, electronic structure and an investigation of charge transfer by multiple charge population analysis approaches was performed.

The work was motivated by the recent experimental observation of adsorption of titanium on graphene which uncovers substantial n-type doping and reduction of graphene's mobility by charged impurity scattering and subsequent recovering of graphene properties to the almost intrinsic values by exposing samples to oxygen [1].

References
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BP19

Search for Resonances in the Dilepton Mass Distribution in Proton-Proton Collisions at sqrt(s) = 7 TeV

L. Thomas, Th. Reis

Université Libre de Bruxelles – IIHE (ULB-VUB)

The theory of particle physics is today described with great accuracy by the Standard Model. However, several important questions are left opened such as the hierarchy problem or the equal number of generations of leptons and quarks. A large number of theories beyond the Standard Model (BSM) have been proposed to answer them and the recent start of the Large Hadron Collider at CERN is expected to allow to test them experimentally. In this poster, we present the search, with the CMS detector at LHC, of new heavy neutral resonances predicted by several BSM theories (Grand Unification, Extra Dimensions,...). The di-electron and di-muon channels are considered. The results on the whole 2011 dataset are presented. The selection and identification of events are described and the efficiency and background contamination are estimated by data driven methods. No evidence of new physics is observed and different limits, depending on the model, are set on the mass of a new heavy resonance.

PARALLEL SESSION (A)

ASTROPHYSICS, GEOPHYSICS & PLASMA PHYSICS

Auditorium D.0.08, 15:00 – 17:30

Chairman: Fabrice Louche (Royal Military Academy)

Invited lecture:

	15:00 – 15:30	"Plasma wall interaction : a key question on the road to a fusion reactor ?"	V. Philips FZ. Juelich, Germany

Contributed Lectures:

A1	15:30 – 15:50	"Solar prominences: formation, force balance issues, and internal dynamics"	R. Keppens K.U. Leuven
A2	15:50 – 16:10	"The formation of type Ia supernovae: theory vs. observation"	N. Mennekens V.U. Brussel
A3	16:10 – 16:30	"Multiple shocks Acceleration & high energy cosmic rays in active galactic nuclei jets"	A. Meli U. Liège
A4	16:30 – 16:50	"Modelling RF sheath dynamics for fusion applications"	D. Van Eester ERM/KMS
A5	16:50 – 17:10	"The Chemical composition of S stars"	P. Neyskens U.L. Bruxelles
A6	17:10 – 17:30	"The PICASSO mission: a Belgian cubesat for the study of the upper atmosphere, the ionosphere, and the magnetosphere of the Earth"	J. De Keyser IASB-BIRA

Plasma wall interaction : a key question on the road to a fusion reactor

V. Philipps

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Forschungszentrum Jülich,
Assoziation EURATOM-FZJ, Trilateral Euregio Cluster, 52425 Jülich, Germany

Fusion energy has the potential of a sustainable and safe energy source with a limited amount of long wasting nuclear waste. After systematic R&D in many fusion labs worldwide, the first fusion device with a net output of energy is being built in South of France, ITER. ITER is the cooperative effort of seven partners, Japan, India, China, Korea, Russsia, EU and US and represents the largest cooperative scientific project ever performed by mankind.

Among the most challenging steps from present fusion devices with low duty cycles towards ITER are questions of plasma wall interaction and selection of wall materials: the control of material erosion and migration (wall lifetime) and the associated long-term tritium retention and the control of plasma instabilities which can damage the first wall if not properly controlled.

This contribution will describe the present status of fusion research, the status of ITER and JET (the present largest fusion device in the world operated by the EU in UK) and the importance of plasma wall interaction and material physics on the way to a commercial fusion reactor.

Solar prominences: formation, force balance issues, and internal dynamics

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Prominences represent fascinating large-scale, cool and dense structures, sus- pended in the hot and tenuous solar corona above magnetic neutral lines. Starting from magnetohydrostatic force balance arguments, their differing magnetic topol- ogydistinguishesKippenhahn–Schlüter(1957)versusKuperus–Raadu(1974)types. In both, the concave-upward parts of magnetic field lines or 'dips' host and support prominence material via the magnetic tension force against gravity.

I will highlight recent insights into prominence physics, where we start from modern magnetohydrodynamic equilibrium computations, allowing to mimick flux- rope embedded multi-layer prominence configurations of Kuperus–Raadu type. These can be analysed for linear stability, and by quantifying the eigenfrequen- cies of flux-surface localized modes, charting out the continuous parts of the MHD spectrum, we pave the way for more detailed prominence seismology.

Perhaps the most elusive aspect of prominence physics is their sudden forma- tion, and we demonstrate recent achievements in both rigid field, and fully multi-dimensional simulation efforts. The link with the thermal instability of optically thin radiative plasmas is clarified, and we show the first evaporation-condensation model study where we can demonstrate how the formed prominence stays in a force balanced state, which can be compared to the original Kippenhahn–Schlüter type magnetohydrostatic model.

The formation of type Ia supernovae: theory vs. observation

Niki Mennekens, Dany Vanbeveren, Jean-Pierre De Greve & Erwin De Donder

Vrije Universiteit Brussel

Type Ia supernovae (SNeIa), the most powerful events in the universe, are critical for cosmology and the chemical evolution of galaxies. They are caused by the thermonuclear explosion of white dwarfs in binary stars, which are no longer able to support themselves due to exceeding a critical mass. The formation mechanism of SNeIa remains unclear: in the single degenerate scenario they form through accumulation of mass given to the white dwarf by its companion star, while in the double degenerate scenario the explosion is caused by two white dwarfs merging. We use a population code including detailed binary star evolution to compute the time range during which SNeIa can occur after the formation of a group of stars. The code allows to differentiate between those physical scenarios and parameters which are still uncertain. These theoretical time distributions are compared to those which are observed, allowing to constrain the physical models. Using a galactic code, a comparison is also made between predictions by different models and the observed metallicity distribution of G-type dwarfs in the solar neighborhood. Because of their very long lifetime, the iron content of these stars is a good indicator of the chemical history, which is critically affected by the rate of SNeIa. We find that neither observation can be theoretically reproduced by the single degenerate scenario alone. The double degenerate one, or especially both scenarios combined, does result in fair agreement, also yielding more knowledge about the exact evolution leading to SNeIa. Including more detailed descriptions of the effects rotation has on the evolution of stars may further close the remaining gap between theory and observation.

Multiple Shock Acceleration & High Energy Cosmic Rays in Active Galactic Nuclei Jets

Athina Meli

IFPA Department of Astrophysics, Geophysics and Oceanography University of Liège Belgium & Web Institute of Physics, www.wiph.org

Shocks in jets and hot spots of Active Galactic Nuclei (AGN) are one prominent class of possible sources of the observed ultra high energy cosmic rays (UHECRs).   It seems implausible that more than at the very best 1/3 of the central black hole power, assuming for example Centaurus A as a main source, goes into the required flux of energetic particles in the jet thus, one would need to allow for the possibility that there is a puzzling source power problem, which we would like to address here. Sequences of consecutive mild relativistic oblique shock features, have been theorized and eventually observed in many AGN jets. Here, we use detailed test-particle Monte Carlo simulations in order to   calculate particle spectra while monitoring the efficiency of the acceleration in consecutive shocks in these jets. We find that consecutive shock patterns of various inclinations push the particle energies up to the UHECR energy regime, rendering flatter energy distributions with steep cut-offs, by leaving a depletion at low energies,   thus the puzzling massive source power mentioned above, would be no longer necessary. Our calculations interestingly show a variation of efficiencies and spectral slopes, connecting to the inclination of shocks to the jet axis, shedding further light into the understanding of irregular or flat gamma-ray or x-ray spectra observed in many AGN jets.

---- Dr. Athina Meli IFPA Institut d'Astrophysique et Géophysique Allée du 6 août, 17 - Bât. B5a B-4000 Liège 1 (Sart-Tilman) Belgium Tel : +32 4 366 34 60 Fax : +32 4 366 36 72 ---

A4 Contributed Lecture Astro-, Geo-, and Plasma- Physics

Modelling RF sheath dynamics for fusion applications

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One of the most efficient ways to heat ions to high temperatures in magnetic confinement fusion machines relies on exciting plasma waves via radio frequency (RF) antennas. Traditional modelling of RF electromagnetic field patterns close to antenna structures is done assuming the plasma density in the antenna box and just in front of it is low enough to allow discarding plasma effects altogether. The effect of the magnetized plasma is only accounted for in the region where the excited waves become propagative. Experimental evidence shows, however, that the plasma directly in front of the antenna and the electromagnetic fields launched by the antenna *do* interact. Accounting for this cross-talk is important for a number of reasons. First of all, the efficiency of the coupling of the externally launched waves to waves that propagate in the plasma and that deposit their power in the plasma core depends on the density profile but at the same time experimental evidence shows that launching of significant amounts of power non- negligibly distorts the plasma edge density. Secondly, since all relevant components of and near to the launcher are made of metal, sheath fields tend to form very close to the walls of the antenna box and the antenna straps. The significant voltage drop across these sheaths can give rise to non-resonant ion acceleration, which is thought to be the source of hot spots and sputtering points close to or on the antenna straps. At these points the metal temperature increases as it is bombarded by a stream of energetic ions. Since plasma purity is essential to reach high temperatures in fusion machines, all processes that give rise to metal ions being released from the vessel and ending up in the main plasma should be characterized to enable reversing or reducing the effect and hence minimizing the pollution of the plasma.

The present work adopts a 2-fluid plasma description approach to describe the interaction of the electromagnetic fields and the particles. The intricate interplay between electric and magnetic field components on the one hand, and the electron and ion densities and velocities on the other hand will be illustrated. Several aspects will be highlighted. In view of the fact that antenna modelling of realistic antenna geometries requires powerful computers both with large memory and high speed processors, the ultimate goal is to assess if the so far used antenna models need to be upgraded or if the essential ingredients of the supplementary physics can be included in a sufficiently accurate but approximate way to avoid compromising the CPU time and memory consumption.

The chemical composition of S stars

Neyskens, P.; Van Eck, S.; Plez, B.; Goriely, S.; Siess, L.; Jorissen, A.

Université Libre de Bruxelles

S-type stars are thought to be the first objects, during their evolution on the asymptotic giant branch (AGB), to experience s-process nucleosynthesis and third dredge-ups, and therefore to exhibit s- process signatures in their atmospheres. Until present, the modeling of these processes is subject to large uncertainties. Precise abundance determinations in S stars are of extreme importance for constraining e.g., the depth and the formation of the 13C pocket. We present a large grid of MARCS model atmospheres for S stars used to derive precise abundances of key s-process elements and iron. A first estimation of the atmospheric parameters is obtained using a set of well- chosen photometric and spectroscopic indices for selecting the best model atmosphere of each S star. Abundances are derived from spectral line synthesis, using the selected model atmosphere. Special interest is paid to technetium, an element without stable isotopes. Its detection in stars is considered as the best possible signature that the star effectively populates the thermally-pulsing AGB (TP-AGB) phase of evolution. The derived Tc/Zr abundances are compared, as a function of the derived [Zr/Fe] overabundances, with AGB stellar model predictions. The computed [Zr/Fe] overabundances are in good agreement with the AGB stellar evolution model predictions, while the Tc/Zr abundances are slightly over-predicted. This discrepancy can help to set stronger constraints on nucleosynthesis and mixing mechanisms in AGB stars.

The PICASSO mission: A Belgian cubesat for the study of the upper atmosphere, the ionosphere, and the magnetosphere of the Earth

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PICASSO is a 3U cubesat project of the Belgian Institute for Space Aeronomy and the Royal Observatory of Belgium. It is planned to fly on the QB50 precursor mission at about 500 km altitude in a high-inclination orbit. PICASSO will host 3 instruments. A spectral imager in the visible-near infrared range (400-800 nm) will observe the Earth's atmospheric limb during orbital solar occultations. By measuring the light absorption in the Chappuis band, vertical profiles of the ozone concentration can be retrieved. Occasional observations of aurora are foreseen with a full spectral scan of the image. A micro-bolometer will measure the radiative flux in selected directions at selected wavelengths to record thermometric and optometric signatures of atmospheric variability. Finally there is also an instrument that is dedicated to plasma physics: a multi-needle Langmuir probe developed by the University of Oslo will assess in-situ the electron density of the plasma at 500 km altitude, which is the transition between the ionosphere and the magnetosphere. We will discuss the characteristics of this instrument and the particular environmental conditions in which it has to operate. We give a brief overview of the science objectives. In particular, we show how coordinated observations with the EISCAT radars in Northern Scandinavia can improve the scientific return from the mission.

Plasma surface impedance matrix and modeling the antennas facing plasmas.

V. Kyrytsya[1], D. Van Eester[1], K. Crombé[1,2], F. Louche[1]

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Although modern commercial antenna codes can handle the complex 3D geometry of ICRF antennas they still can not correctly describe hot fusion plasmas. In view of the impact the plasma has on the antenna-near fields and hence the need to use a sensible mock-up for the plasma behavior, ICRF antenna modeling is currently mostly done by substituting the plasma with suitably chosen dielectric [1,2]. One of the limitations of this approach is the incorrect evaluation of the fields on the plasma surface.

In this work a theoretical basis is given and a practical implementation is shown for coupling the spectral plasma surface impedance matrix [3] to modern commercial antenna codes for self-consistent correct calculation of the fields and scattering ('S') parameters of the ICRF antennas, hereby allowing to interface the antenna coupling code with a much more realistic model for capturing the subtleties of magnetized plasmas. The approach uses subsequent application of induction and uniqueness theorems of electromagnetism. In a first step the fields of the antenna in vacuum are computed. Once these incident fields are known one can use the surface impedance of the plasma to calculate the total electric and magnetic fields on the plasma surface and the power flow into the plasma. The evaluation of the S-parameters of the antenna requires a second step. We use the obtained tangential electric field on the plasma surface as a necessary boundary condition to solve the equivalent problem and find the S-parameters of the antenna and all the fields around it.

This new approach is similar in physics potential to the TOPICA code [4] for its application to antenna design for fusion machine applications; to date TOPICA is the most advanced academic antenna code for 3D ICRF antennas modeling. Moreover, it is possible to simulate the presence of cold low density plasma in the antenna box, which is needed for the correct evaluation of the fields and for addressing the sheath effect. The here presented, new approach is numerically more efficient and user-friendly than codes that attempt to directly incorporate the plasma response in the antenna computation. The paper also compares results obtained using the new approach with those obtained by other modeling methods.

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Fusion product measurements in TEXTOR tokamak plasmas using activation technique

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MeV particle loss measurements from fusion plasmas, in particular alpha particles, remain difficult in large fusion devices and further R&D is needed for ITER[1-2] and future fusion reactors. This paper describes the first attempt to measure fusion-reaction protons emitted from TEXTOR tokamak plasmas using a new plasma diagnostic technique. This new measurement technique was successfully demonstrated, initially, in 2006 on the large JET tokamak[3]. A small ion camera equipped with a collimator and several types of activation detectors was installed inside the TEXTOR vacuum vessel to perform these measurements. New detector materials were tested including a highly pure (9N) germanium detector 87.6% isotopically enriched in ^{76}Ge, a promising candidate for an alpha particle detector for ITER. After the irradiation, the detectors were removed and analyzed using ultra low level gamma ray spectrometry[4] in HADES underground laboratory at IRMM, Belgium. 3 MeV escaping fusion-reaction protons were detected in larger number - ~ 6 times more - compared to earlier measurements using this technique on JET. Another major progress was the reduction of the cooling time by a factor 50 which made possible to detect radionuclides with half-life of less than 90 minutes.

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Non-thermal velocity distribution functions in space plasmas

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Suprathermal particle distributions are ubiquitous at high altitudes in the solar wind and many space plasmas, their presence being widely confirmed by spacecraft measurements. The presence of non-thermal populations in space plasmas has important consequences concerning particle acceleration and plasma heating. These effects are well described by the kinetic approach where the suprathermal tails can be represented by different velocity distribution functions such as a sum of two Maxwellians with different temperatures or, better, with a Kappa distribution decreasing as a power law of the velocity (Pierrard and Lazar, 2010).

Recent results obtained in the development of space plasma kinetic models are presented. They concern the solar wind and corona, planetary magnetospheres and auroral regions. We show how the solution of the evolution equation is used to determine the velocity distribution function of the plasma particles and their moments. The solutions depend on the approximations and assumptions made in the development of the models. We describe in particular the results obtained with the collisionless exospheric approximation, the effects of Coulomb collisions obtained by using a Fokker-Planck term in the evolution equation, the effects of wave turbulence for the electrons and those of kinetic Alfvén waves for the generation of beams in proton distributions [2].

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Links between the plasmapause and the radiation belt boundaries from Cluster measurements

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The radiation belt dynamics is strongly influenced by the core plasmasphere distribution and, more specifically, by the position of the plasmapause. The plasma content in the plasmasphere and the position of the radiation belts are studied on the basis of recent CLUSTER observations, when the spacecraft perigee was as close as L=2. Density profiles along the spacecraft orbit can be derived from the plasma frequency line determined from the WHISPER wave observations. From these, the plasmapause position can be derived. The radiation belt positions can be determined from a careful analysis of the background noise in the CIS data, but also with the high-energy RAPID spectrometers. We compare the plasmapause and radiation belt positions and discuss their relation.

The dynamics of the Earth's inner magnetosphere

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Solar storm events have a huge effect on the Earth's inner magnetosphere. The inner magnetosphere contains charged particles trapped in the magnetic field of the Earth and coming from the ionosphere, the plasmasphere and the radiation belts. The ionosphere is the part of the upper atmosphere that becomes ionized due to the solar radiation. It is located from a height of 50 km to 1000 km. The plasmasphere is the extension of the ionosphere at higher altitudes and is filled by these cold ionospheric particles. A three dimensional physical dynamic model of the plasmasphere has been developed at BISA and has recently been coupled to the IRI (International Reference Ionosphere) model [1].
Dynamical simulations of the plasmasphere model can be run on the space weather portal (www.spaceweather.eu) and on the CCMC website of NASA (http://ccmc.gsfc.nasa.gov).

The radiation belts contain very energetic electrons and protons. Based on the empirical fluxes of the AP8-MIN and MAX NASA model, we have determined with a kinetic approach the density and energy description of the proton populations [2]. Based on CLUSTER satellite measurements, an empirical three dimensional dynamic model of the radiation belts is also in development. This model forecasts the dynamics of the radiation belts based on the predicted Dst (disturbed storm time) index.

[1] Pierrard V. and K. Borremans, The ionosphere coupled to the plasmasphere and polar wind models, Astronum2011 Proceedings, ASP Conference series, 2012 a
[2] Pierrard V. and K. Borremans, Fitting the AP8 spectra to determine the proton momentum distribution functions in space radiations, in press in Rad. Meas., 2012b

COMPUTATIONAL STUDY OF THE GRAD - SHAFRANOV EQUATION IN HELICAL SYMMETRY

Lorenzo Siddi1 Luca Guazzotto2 Giovanni Lapenta3

We present here a numerical solution of the Grad - Shafranov equation in cylinder geometry. The main challenge is the full inclusion of helical symmetry, a problem relevant in a variaty of scenarios. Cylindrical geometry can be a first step for the solution of Grad - Shafranov equation in Tokamak. But in many other situations in laboratory and astrophysical plasmas, an helical symmetry is more approriate.
The Grad - Shafranov equation is solved with a helicoidal symmetry with a convective term expressed by toroidal and poloidal velocities. We thus obtain a coupled system: a non-linear Poisson equation for the magnetic flux $\Psi(r, u)$ and a Bernoulli equation for the density $\rho(r, u, \Psi)$:

$$\frac{1}{2}\left(\frac{\Phi B}{\rho}\right)^2 - \frac{1}{2}\left(\frac{\Omega(\Psi)}{h}\right)^2 + W = H(\Psi)$$

$$\nabla \cdot \left[\left(1 - \frac{\Phi^2}{\rho}\right) h^2 \nabla\Psi\right] = f(r, u, \Psi)$$

(1)

Here, we report our progress in the development of a numerical method and computational code to solve the coupled non-linear system (1). Our numerical treatment is first tested with analytical equilibrium solutions (Solov'ev equilibra). Example of application will be described.

Investigation of geometrical evolution in 3DPIC simulation of an infinite flux rope

Anna Lisa Restante, Stefano Markidis, Giovanni Lapenta

Katholieke Universiteit Leuven

In plasma physics and solar physics one of the studied key structures is the flux rope as a simplification and generalisation of real events. The understanding of their evolution through 3D simulation is one of our main goals. In this presentation we would like to describe our last study on this topic, in particular we have been investigating a kinetic simulation of kink instability in an infinite flux rope. We have investigated the evolution of its geometry considering various techniques such as Poincare' maps and Quasi-Seperatrix Layer (QSL). QSL's, in particular have been used by solar physicists to estimate regions in which 3D magnetic field line reconnection may occur and consequently where heating and current can generate.

PARALLEL SESSION (B)

ATOMICS, MOLECULES OPTICS & PHOTONICS

Auditorium D.0.07, 15:00 – 17:30

Chairman: Xavier Urbain (Université Catholique de Louvain)

Invited lecture:

	15:00 – 15:45	"High harmonic spectroscopy: from electron tunneling to molecular dynamics"	B. Fabre CELIA, Université de Bordeaux I
	15:45 – 16:30	"Micro-Photonics at the Brussels Photonics Team"	H. Ottevaere V.U.Brussel

Contributed Lectures:

B1	16:30 – 16:45	"Casting light on the darkening of colours in historical paintings"	F. Da Pieve Univ. Antwerpen
B2	16:45 – 17:00	"Probing trap depths in persistent phosphors"	K. Van den Eeckhout Univ. of Ghent
B3	17:00 – 17:15	"High sensitivity of the optical response of porous natural photonic structures to the presence of gases and vapours"	S. Mouchet FUNDP Namur
B4	17:15 – 17:30	"Thermal conductivity depth profiling of hardened solids using infrared photothermal radiometry technique based on artificial neural network recognition"	Liwang Liu K.U. Leuven

High harmonic spectroscopy: from electron tunneling to molecular dynamics

Baptiste Fabre
CELIA, Université de Bordeaux I

Electron scattering is one of the main tools to probe the structure of matter. It has been successfully used to resolve the structure of solids, molecular, and biological complexes. Recent advances in strong field light-matter interactions have opened a window into a new class of phenomena where electron scattering is initiated and manipulated by strong laser fields. In these experiments, the strong field leads to tunnel ionization which splits the electronic wave function into two parts: a bound state, associated with the hole left behind the escaping electron, and a continuum state. The free part of the electron wave packet is accelerated in the laser field and can recollide with the parent ion. Recollision can lead to the emission of optical radiation. This process is known as high-order harmonic generation.

Due to their remarkable spatial and temporal characteristics, high harmonics are nowadays used as valuable spectroscopic tool. Two different experimental schemes are mainly developed:

* VUV spectroscopy where high harmonics are focalized on the studied system (atomic or molecular) in a spectrometer (velocity map imaging spectrometer, time-of-flight spectrometer...). In that case, information about the system is obtained by collecting electrons or ions produced by the interaction with the harmonic beam.

* Extreme Non-Linear Optical Spectroscopy (ENLOS) where high order harmonics are directly generated into the studied system. Spectroscopic information is then directly encoded into the High Harmonic spectrum properties (amplitude, phase, polarization...)

During this talk, applications of each of these spectroscopies developed either in the CELIA laboratory (University of Bordeaux 1) or during international collaborations will be presented. In a first part, we will focus on an experiment in which we applied the RABBITT method (2-color 2-photon ionization used normally to recover the relative phase between two consecutive harmonics) in an original way to study the near-threshold photoionization of N2. By combining these measurements with a theoretical model we were able to reveal the delay associated to the ionization and the effect of resonances on this process. In a second part, we will concentrate on the ENLOS spectroscopy and its ability to recover structural information on the generating medium. In particular, we will put in evidence the role of the ionic potential which influence is generally neglected, most of the studies being done in the Strong field approximation framework. Thus, we have developed a semi-classical model, called CTMC-QUEST (Classical Trajectory Monte-Carlo QUantum Electron Scattering Theory), which allows us to simulate the high harmonic generation and understand the role of experimental parameters on this process. This model is used to interpret several experiments such as:

* Cooper minimum in Argon
* Polarimetry in Argon : study of Coulomb focusing
* HHG in chiral medium : circular dichroism

Finally, in a last part, we will apply ENLOS spectroscopy to study the NO2 dynamics close to a conical intersection. Experimental results will be compared to semi-classical Trajectory Surface Hopping simulations. This experiment highlights the HHG sensitivity to instantaneous electronic configuration of the molecule.

Invited Lecture Atoms, Molecules, Optics and Photonics

Micro-Photonics at the Brussels Photonics Team

Heidi Ottevaere

Department of Applied Physics and Photonics TONA
VUB, Vrije Universiteit Brussel

Photonics -the "Science-and-Technology-to-Harness-Light"- is a discipline that involves fundamental research of photons, of light-matter interactions, and the development of novel technologies and applications based on the unique properties of light. Photonics leverages these unique properties to probe, sense, transmit, process, display and store information, and to accomplish a multitude of original functionalities, which cannot be achieved otherwise.

The Brussels Photonics team (B-PHOT), under the leadership of Prof. Hugo Thienpont, has been active in the field of micro-photonics for more than 20 years. With its micro-optical design platform, its cyclotron based deep-proton writing, and its large-scale micro-optical measurement centre in clean room conditions B-PHOT is currently among the world-leaders in optical modeling, optical characterization, low-cost rapid prototyping, and proof-of-concept demonstration of micro-optical modules and has research collaboration agreements with top-level research groups in Europe, in the United States, Australia, and Asia. At the conference we will elaborate on the recent scientific achievements and touch upon the research plan that B-PHOT intends to develop during the next years to continue to push the frontiers of microphotonics research.

Casting light on the darkening of colours in historical paintings

F. Da Pieve [(1)], C. Hogan [(2,3)], D. Lamoen [(1)], J. Verbeeck [(1)], K. Janssens [(4)],
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(1) EMAT, Department of Physics, University of Antwerpen, Antwerpen, Belgium
(2) Italian Research Council, CNR, Rome, Italy
(3) ETSF, European Theoretical Spectroscopy Facility
(4) Department of Chemistry, University of Antwerpen, Antwerpen, Belgium
(5) Unité NAPS, Catholic University of Louvain, Louvain La Neuve, Belgium

In recent years, the colour evolution of pigments in several historical paintings belonging to our archaeological and artistic heritage over the world has triggered an intense experimental effort based on X-ray and microscopy techniques. Several works on the blackening of vermillion (α-HgS, often called cinnabar) demonstrate that the colour change is a complex phenomenon rather than a single step process, and is related to the formation of different chemical species, like corderoite
(α-$Hg_3S_2Cl_2$), calomel (Hg_2Cl_2) and mercuric chloride ($HgCl_2$) [1,2,3]. Various routes for degradation of red cinnabar have been proposed, but the origin of the permanent photodarkening of cinnabar and its full transformation sequence remain a mystery for scientists and conservators. A variety of properties affect the transformation, including the band gap for photon absorption of the compounds, their band edge positions and stability. Such colour change phenomena constitutes a fascinating challenge for our fundamental understanding of light-matter interaction through first-principles theories, which aim at describing physical and chemical phenomena without any input parameters from experiments. From the fundamental point of view, the description of light-matter interaction in a band approach often requires advanced theoretical methods, beyond the widely used ab-initio density functional theory (DFT), currently an invaluable tool for computing ground state properties in materials science, chemistry and biology. Among such advanced methods, many body perturbation theory (MBPT) [5,6] is a first principles many-electron Green's function approach which has yielded excellent predictions of spectroscopic properties for a wide class of materials . Here we demonstrate that state-of-the-art theoretical spectroscopy based on the combination of DFT and MBPT is able to unravel the complex origin of the darkening of cinnabar and that a critical re-examination of some hypotheses previously suggested from experiments is needed. We analyze the X-ray and visible light response of the main compounds observed in experiments on degraded paintings, we explain the photoactivation of the cinnabar surface and we identify the defective structures which act as chromophoric groups in the uppermost layers and are responsible for the discolouration process.

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Probing trap depths in persistent phosphors

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Contrary to most luminescent materials, persistent phosphors can continue emitting light for hours after being excited. It is generally agreed upon that excited electrons can escape the luminescent centers and get caught by so-called 'traps' in this kind of materials. A certain activation energy, or 'trap depth', needs to be overcome before the electrons can return to the luminescent centers and produce light. Unfortunately, the nature of these traps and the kinetics of the trapping/detrapping process remain the subject of debate [1]. Therefore, the development of better and brighter persistent phosphors, strongly desired for emergency signage and medical imaging, remains a process of trial-and-error.

An effective and versatile approach to study the trap structure in persistent phosphors is thermoluminescence. By heating a previously excited material and simultaneously monitoring the emitted light, information on the trap depths and the trapping kinetics can be deduced. Using this technique, we were able to prove the presence of a continuous trap distribution in the blue-emitting persistent phosphor $CaAl_2O_4$:Eu,Nd. Furthermore, we will discuss the major pitfalls when using thermoluminescence for studying the trapping processes in persistent luminescent materials, and how they can be avoided.

[1] K. Van den Eeckhout, P. F. Smet, D. Poelman, Materials 3 (2010), 2536-2566

High sensitivity of the optical response of porous natural photonic structures to the presence of gases and vapours

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Structurally coloured natural photonic crystals (found in butterflies, beetles and other insects) are made of ordered porous chitin structures. In such photonic crystals, colour changes can be induced by relative gas/vapour concentration variations in a mixed atmosphere. For instance, when the composition of the atmosphere changes, the colour of Morpho sulkowskyi butterfly is modified [1]. Based on this effect, Potyrailo and coworkers demonstrated experimentally the possibility to identify closely related vapours [1]. They explained their observations by the occurrence of different spatial periodicities in the nanostructures from different regions of the butterfly wing: different photonic crystal periods are thought to be responsible for the wavelength selective optical response [1]. Recently, Biró and coworkers investigated four butterfly species and demonstrated fast, reproducible species-dependent selective sensitivity to seven test vapours [2].

In spite of increasing interests for such sensors, the fundamental mechanisms at the origin of the selective optical response are still not well understood.

The point is that refractive index variations resulting from the introduction of a specific gas species in the atmosphere are too small to justify entirely the dramatic changes observed in the optical response. Here, we demonstrate through numerical simulations that indeed gas/vapour-induced refractive index changes (typically $\Delta n \approx 10^{-6} - 10^{-7}$ between dry air and 50% relative humidity water vapour) are too small to produce a significant modification of the spectral reflectance in a representative 3D periodic model of natural porous nanostructures. For this purpose, we used a rigorous coupled wave analysis method for modelling light scattering from inhomogeneous optical media. The origin of the reported colour changes has therefore to be found in chemical modifications of the porous material and their impact on the photonic response.

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B4 Contributed Lecture Atoms, Molecules, Optics and Photonics

Thermal conductivity depth profiling of hardened solids using infrared photothermal radiometry technique based on artificial neural network recognition

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The thermal conductivity of materials, very sensitive to heterogeneities, is a quite appropriate thermophysical quantity to probe their microstructure. Laser induced Photothermal radiometry (PTR), based on the generation and detection of thermal waves in the sample being detected, has become a powerful tool for the thermophysical characterization of broad classes of materials, due to its non-destructive and highly sensitive nature. In this paper, we focus on hardened steel samples, in which a depth profile of varying microstructure is induced by a hardening treatment. An artificial neural network recognition approach is used to extract the thermal conductivity depth profile from PTR signals obtained in a non-contact way on flat and cylindrical steel rods. The quality of the reconstructed thermal conductivity depth profile is confirmed by a good correspondence between the signals calculated a posteriori from the profile and the experimental data that were fed to the neural network. The results confirm the expected anti-correlation between the thermal conductivity and the hardness, which was determined from a classical indentation procedure at different depths.

B5 Poster, Molecules, Optics and Photonics

Imaging ellipsometry : a multivariate analysis strategy based on **k**-means and hierarchical clustering for fast data inversion*

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Ellipsometry is a well-known non-destructive analysis technique used to determine the optical properties of materials as well as the coating thickness in an optical stack. The method is based on the change of the polarization state of a light beam after the reflection at the sample surface. One defines the ellipticity r as the ratio of the reflection coefficients **Rp** and **Rs** which are the **p**- and the **s**- components of the electrical field associated to the light wave :

$$\rho = \frac{R_p}{R_s} = \tan\Psi e^{i\Delta} \text{ with } \tan\Psi = \frac{|R_p|}{|R_s|} \text{ and } \Delta = \delta_p - \delta_s$$

This relation also defines the ellipsometric angles **Y** and **D**. Theses ellipsometric angles are usually interpreted on the basis of an optical model, assuming sharp interfaces between the different layers of the sample. From the experimental point of view, the optical and structural parameters are averaged over the beam size whose small axis (lateral resolution) is typically of the order of 2–4 millimeters for parallel beam configurations or of 50–100 micrometers when focusing optics are used. One possibility to access to the local optical properties at the (sub-)micron scale is to consider imaging ellipsometry, a technique which yields images of the ellipsometric parameters (**Y** and **D** maps). In that case, the lateral resolution is approximatively 1 mm. The drawback of having a high lateral resolution is that the amount of data to be inverted using non-linear fitting algorithms tremendously increases.

In this paper, we consider two-steps statistical algorithms to identify the pixels of the image characterizing regions of the sample having a similar optical response. Typically, 128 or 256 regions are selected and the ellipsometric equations are numerically solved for each of them. The solution is back-propagated on the initial images to get a thickness or a refractive index map. This procedure considerably decreases the processing time of the data. Examples concerning SiO2 on Si samples, with (Fig. 1A and 1B) and without patterns, will be given as well as simulations results.
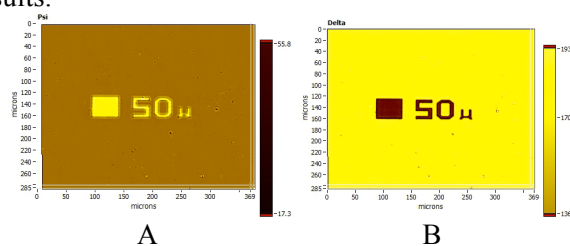

Figure 1 : (A) **Y** and (B) **D** maps of a ' 100nm-thick SiO2 pattern on a native oxide background (pattern size : 50 mm, Magnif. : 10 _)

Spectroscopy visualization of acoustic clapping with photorefractive interferometry

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Nonlinear acoustic methods have demonstrated high potential in recent years in the field of nondestructive testing (NDT) due to their enhanced sensitivity and especially their "defect selective" behavior. Many defects in materials involve nonbonded surfaces which causes contact acoustic non-linearity (CAN). Higher harmonics of the frequency of the driving harmonic vibration can be generated through two mechanisms; energy dissipation due to the tangential friction of the boundaries and "mechanical rectification" due to interface clapping. Several full-field imaging techniques have been implemented to exploit the potential of this effect, including shearography [1] and scanning laser Doppler vibrometry [2]. While shearography is subject to a complex relation between the interferograms and the acoustic displacement, namely non-straightforward interpretation of the results, scanning laser Doppler vibrometer needs to compromise between optimum spatial resolution and speed of operation. In this paper, a photorefractive interferometry method [3] is elaborated to visualize nonlinear acoustic phenomenona while overcoming the disadvantages in the above mentioned techniques. As a proof of concept, a PVDF film is harmonically excited, with a metal tip touching its surface, which creates the "mechanical rectification" and higher harmonics of the excitation frequency arise at the location of the clapping. By utilizing the narrow-band feature of the photorefractive crystal, and mixing down the frequency of vibration patterns by choosing a proper phasemodulation frequency of the reference beam of the interferometer, vibration components of interest, e.g. higher harmonics due to "mechanical rectification", can be selectively imaged, while disturbing optical effects due to the strong vibration component of the excitation frequency are suppressed. This results in outstanding performance on detection of acoustic nonlinearity in the presence of strong background linear acoustic motions. Acoustic nonlinearity can be imaged without scanning by providing a full-field interferogram with the intensity of each pixel directly proportional to the displacement amplitude at the corresponding point on the sample surface. Absolute measurement of the surface dynamics can be performed with micrometer resolution in the imaging plane and in depth.

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B7 [BP8] Poster, Molecules, Optics and Photonics

Saturated green phosphors for LED applications

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Solid state light sources possess several advantages over traditional light sources (like incandescent or fluorescent lamps), including a long lifetime, high efficiency, small footprint and the absence of toxic substances. While for general lighting applications a wide emission spectrum is preferred to increase the colour rendering, display applications require light sources with a saturated emission colour [1]. In this work, we explore green luminescent materials which can efficiently convert the emission from a blue light emitting diode (LED). First a variety of phosphors hosts (including $SrSi_2O_2N_2$, $Ba_3Si_6O_{12}N_2$, $ZnGa_2S_4$ and $SrGa_2S_4$) are doped with divalent europium, and evaluated in terms of luminescence properties, thermal quenching and efficiency.

Then $Sr_{1-x}Eu_xGa_2S_4$ phosphors are studied in more detail over a wide dopant concentration range ($x = 0.01$ to 0.3), as function of temperature. The phosphors show a saturated green emission, with a peak wavelength around 536nm and a FWHM of 50nm. The internal quantum efficiency is 71% for $x = 0.04$. For this concentration, the emission intensity at 400K is still 90% of the intensity at room temperature. By measuring decay and thermal quenching profiles as a function of europium concentration, we were able to explain the emission properties on the basis of the local environment of the europium ions in the lattice [2].

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Beating the diffraction limit in the subwavelength confinement of light using radial and azimuthal transformations of the electromagnetic space

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The confinement of electromagnetic energy is an essential ingredient in studies of the quantum mechanical properties of light as well as in several applications involving the storage and manipulation of information. A common way to achieve this is the use of optical resonators, in which light is held by internal reflection on its boundaries. However, due to the wavelike nature of light, it is believed to be impossible to confine light efficiently if the dimensions of the resonator are smaller than the wavelength.
Here we have developed a novel approach to create optical resonators by applying the geometrical technique of transformation optics. Starting from the invisibility cloak, we calculate the bound modes of several cylindrical structures in which light is smoothly guided along a prescribed trajectory. We show that the fundamental diffraction limit can be overcome. Moreover, we generalize this approach by considering more intricate transformations, involving the radial and azimuthal coordinates, that simplify the resulting material parameters. These findings may have wide implications for the storage and manipulation of optical information as well as studies of the fundamental properties of light.

B9 Poster, Molecules, Optics and Photonics

Action spectroscopy to investigate the optical absorption spectra of small gold-palladium cluster cations

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We used the action spectroscopy technique that combines wavelength dependent Xe messenger atom photodetachment and mass spectrometry to investigate the electronic excitation spectra of Au and bimetallic Au-Pd cluster cations. The optical absorption spectra of pure Au_n and Pd doped $Au_{n-1}Pd$ cluster cations ($16 \leq n \leq 20$) were measured in the gas phase by use of the corresponding cluster-Xe complexes in the photon energy range of $1.8 - 5$ eV. The influence of the Pd dopant atom on the optical spectra of the Au_n clusters, which form hollow cages (n = 16-18) [1] and a highly stable tetrahedron (n = 20) [2] is discussed. In addition, the geometry change for the larger cluster sizes (Au_n and $Au_{n-1}Pd$, n > 20) is clearly demonstrated via their ability to attach Xe atoms. Analogical change in the cluster ability to attach Ar atoms was readily observed at 2D-3D transition of pure Au clusters.

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Elastic parameters of a thin (300nm) NiMnGa coating

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Impulsive stimulated scattering (ISS) is an all optical technique that allows to simultaneously investigate the thermal and elastic properties of a material. In the reflection configuration, using a diffraction grating and imaging optics, a pulsed pump laser beam is split into two first orders and recombined at the sample surface thus creating an interference pattern. The energy is delivered in a very short time and the sample thermally expands launching spatially periodic acoustical waves. The dynamically diffracted component of a second CW probe laser beam is used to detect the surface acoustic waves and thermal expansion pattern.

Up to now the technique has been used to investigate, int. al., thin films, multi-layered structures, bulk fluids and fluids at an interface with a solid. In this report the technique is used to investigate a thin layer of NiMnGa on an anisotropic MgO substrate. NiMnGa is a Heusler alloy that has received increased attention because of its magnetic shape memory effect and because of elastic strains of up to 10%. Several authors have reported values for the stiffness parameters of NiMnGa in the austenite phase. In this report we investigate the elastic properties of this material in the, low temperature, martensite phase. The experimental results are analyzed in the framework of a theoretical model for surface acoustic wave propagation in an anisotropic 1D layered medium.

Enhanced sensitivity electro optic measurements for electric fields using an asymmetric Fabry-Pérot cavity

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We provide a new method for high sensitivity measurements of high frequency electric fields with an electro optic crystal. The innovation is the use of a Fabry Perot cavity in order to improve the sensitivity of the method in the high frequency range.

In a first version, measurements were done with a heterodyne detection method. The setup consisted of an electro optic crystal and an acousto optic crystal placed each in one arm of an interferometer. The external electric field to be measured was created by an antenna placed right next to the electro optic crystal which served as a measuring probe. The role of the acousto optic crystal was to shift the measurements frequency by ωS in order to avoid all noises. The signal was then modulated at a frequency ωRF varying between a few kHz and 10 GHz and measurements were performed at a frequency ($\omega RF - \omega S$) by heterodyne down conversion. Electric fields of about 1 V/m were possible to detect.

The new idea is to place the electro-optical crystal inside a Fabry Perot cavity. Hence, the multi passage of laser light inside the electro optic crystal gives us a significant gain factor. In practice, the electo-optic crystal replaces one of the mirrors of the cavity. Measurements with the cavity are already done at frequencies of few tens of kHz. A gain factor of 35 was observed. The next step is to go up to the RF range. But when the round trip of light inside the cavity is not negligible with respect to the period of the external electric field, a gain can still be achieved provided that the round trip is a multiple of the period of the electric field. For example with a 2.5 cm long cavity, the frequency to be measured must be a multiple of 6GHz. The limitation is the bandwidth of the photodetector and not the round trip period or the mean time spent by light inside the cavity.

Optical measurements and ray tracing simulations of LED luminaires with a diffuse ceramic reflector

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A ceramic material with a very high reflectance that is almost perfectly Lambertian was recently developed by a Dutch company. The material is available in two forms: Cerflex®TECH in which the entire bulk of the ceramic has the same optical properties and Cerflex®TECH coating where the optical grade ceramic is a coating on top of a more classic ceramic. A possible application of the ceramic coating material are diffuse reflectors for lighting applications.

In this work a number of simple prototype luminaires with diffuse ceramic reflectors are studied. A ray tracing model of luminaires with a ceramic reflector is constructed and validated by comparing experimentally determined optical characteristics with simulated optical characteristics. The optical characteristics of several luminaires with ceramic reflectors are measured with a near field goniophotometer. These measurements are compared to ray tracing simulations that have the optical properties of the luminaire components as input data.

The simulations are performed with the software package TracePro®. The relevant optical surface properties of the reflector material, the Bidirectional Scatter Distribution Function (BSDF) and the total reflection, are determined experimentally. A ray tracing source model of the LED is constructed from near field goniophotometer measurements. The ray tracing simulations of the luminaires take into account the source model of the LED, the optical properties of the ceramic coating and the geometry of the reflectors. From the simulations it is found that the radiation pattern of this type of luminaire is constructed in a way that is the opposite of the construction of the radiation pattern of a luminaire with a specular reflector.

A remote phosphor LED module with a ceramic mixing chamber: optical measurements and ray tracing

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In the lighting industry it is widely accepted that remote phosphor technology is a key technology for the future of LED lighting. A remote phosphor module consists of a number of LEDs that emit blue light into a mixing chamber, the exit of the chamber is covered with a glass or plastic plate covered with a fluorescent material that transforms the blue light into white light. This way, a white diffuse light source is created of which the performance is not sensitive to imperfections of a LED or random differences between the LEDs.

In this work the optical performance of a remote phosphor module with a classic cylindrical mixing chamber constructed from MPET is compared with the performance of a module with a mixing chamber constructed from a new highly reflective ceramic material (Cerflex®TECH). The near field and the radiation pattern of both modules and of the LEDs is experimentally determined by means of near field goniophotometer measurements. The Bidirectional Reflection Distribution Function (BRDF) of the construction material of the classic and the ceramic mixing chambers is measured. The BRDF is a five variable function that models the scattering of light by a material surface.. The glass plate with the fluorescent material is modeled by means of an extended, six variable, BSDF (Bidirectional Scattering Distribution Function): four variables model the directions of the incident and scattered light and two variables are the illumination and scattered (fluorescent) wavelength. A ray tracing simulation with the BRDFs and the measured optical properties of the LEDs and the phosphor layer as input data is performed using a commercial Monte Carlo ray tracing software package (TracePro®). It is found that the light flux of the module with the ceramic material is higher than the flux of the classical one. There is little difference in the radiation pattern of the modules despite the fact that the BRDF of Cerflex®TECH and MPET are clearly different. The ray tracing simulation can predict the performance of the remote phosphor modules qualitatively, the main difficulty here is in the modeling of the fluorescence.

B14 Poster, Molecules, Optics and Photonics

Electron-impact ionization and dissociation of OH$^+$ and OD$^+$

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Absolute cross section measurements are reported for electron impact ionization and dissociation of Oh$^+$ and OD$^+$ to OH^{2+} and to the D$^+$, O$^+$, O^{2+} and O^{3+} ionic fragments. The electron energy range extends continuously from the threshold of the initial reaction (excitation or ionization) up to 2.5 keV. The ion beam is produced in an ECR ion source, filled with H$_2$O or D$_2$O and accelerated to 10 keV. After magnetic selection, the primary ion beam crosses the electron beam. A 90° magnetic analyzer separates product ions from the primary beam. A magnetic field scan allows the determination of the kinetic energy release (KER) distribution of fragments, for a given incident electron energy [4].

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Quadrupole transitions in the bound rotational-vibrational spectrum of the hydrogen molecular ion

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The three-body Schrödinger equation of the H2+ hydrogen molecular ion with Coulomb potentials is solved in perimetric coordinates using the Lagrange mesh method. Energies and wave functions of up to four of the lowest vibrational bound or quasibound states for total orbital momenta from 0 to 40 are presented. The obtained energies have an accuracy varying from about 13 digits for the lowest vibrational state to at least 9 digits for the third vibrational excited state. With the corresponding wave functions, a simple calculation using the associated Gauss quadrature provides accurate quadrupole transition probabilities per time unit between those states over the whole rotational bands.

Rotationally resolved predissociation lifetimes of the c $^3\Pi_u{}^+$ state of D$_2$

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The c $^3\Pi_u{}^+$ state of molecular hydrogen is subject to rotational predissociation to the repulsive b $^3\Sigma_u{}^+$ state, yielding a pair of ground state atoms. This process is hindered by the poor Franck-Condon overlap with the vibrational continuum of the dissociative state, resulting in lifetimes of the order of 10 to 100ns for the lower rotational levels of the c $^3\Pi_u{}^+$ vibrational ground state of the D$_2$ molecule, as predicted by Comtet and De Bruijn [1].

In order to restrict the population to a few rovibrational levels, a (3+1) REMPI scheme involving the C $^1\Pi_u$ state is applied to create D$_2{}^+$ ions in specified v^+, N^+ levels. These ions are accelerated and formed into a 2 keV beam, that crosses at right angle an effusive potassium beam emerging from a capillary array. The resonant capture of an electron from an alkali target allows for an efficient population of the a $^3\Sigma_g{}^+$ and c $^3\Pi_u$ states. The dissociation products fly apart and strike a pair of position and time sensitive detectors operating in coincidence. This time and position information univocally determines the total kinetic energy released in the process, provided the location of the dissociation is known.

The predissociation lifetime causes the dissociation to occur further downstream, hence the KER to be underestimated, producing a low-energy tail in the spectrum. A full analysis has been performed that incorporates both the exact energy and predissociation lifetimes of specific rovibrational levels. Combined with the known selectivity of the REMPI process [2], these spectra indicate a strong propensity for the charge transfer to populate the c $^3\Pi_u$ state with J=N+ ± 1, pointing to the induced-dipole character of the charge transfer process [3].

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Early crack detection in vibrating structures with piezo-excited and detected acoustic waves.

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Detection of the presence of cracks in materials has always been an important branch of investigation and many different non-destructive testing (NDT) techniques have been developed. The drawbacks of most of the current NDT techniques are that they are only off-line available and that are not able to detect closed cracks. A limitation to off-line detection leads to out of service time and so increases the life cycle cost. The early detection of closed cracks is particularly difficult since ultrasonic waves will travel through this region without linear interaction. This asks for a more specific procedure in which the defects are opened, inducing nonlinear responses. Different nonlinear techniques have successfully been developed but practical implementation is, due to size and cost, still very limited. The methods that can be implemented suffer from a lack of region selectivity and many sources of nonlinear- or nonlinear-mimicking-signal prevent defect detection.

On this poster we will present the current results of the development of a technique in which region selectivity will be exploited by making use of short signal bursts and time-gated detection. Region selectivity avoids reflections and permits Lamb-mode selection. The natural vibrations present in the structure during its operation are a key factor in this concept. The applied stresses in the structure will open and close early cracks, inducing non-linear effects on the probe signal. When a closed crack is present this non-linear interaction with the probe signal will be correlated to the low frequency vibrations in the structure and thus giving a signature of the crack. The modulation of the high frequency probe signal is investigated with lock-in detection, revealing the changes in amplitude due to changed transmission at the crack.

PARALLEL SESSION (C)

CONDENSED MATTER AND NANOSTRUCTURE PHYSICS

Auditorium QC, 15:00 – 17:30

Chairman: François Peeters (Universiteit Antwerpen)

Invited lecture:

	15:00 – 15:50	"Graphene as a prototype membrane: Ripples, puddles and strain engineering"	M. Katsnelson Radbound Univ. Nijmegen

Contributed Lectures:

C1	15:50 – 16:05	"Electronic properties and STM images of N and B doped graphene"	L. Henrard FUNDP Namur
C2	16:05 – 16:20	"Effect of nonhomogenous dielectric background on the plasmon modes in graphene double-layer structures at finite temperatures "	S. M. Badalyan Univ. Antwerpen
C3	16:20 – 16:35	"Thermal conductivity depth profiling of hardened solids using infrared photothermal radiometry technique based on neural artificial network recognition"	L. Liu K.U. Leuven
C4	16:35 – 16:50	"Lattice location of transition metals in dilute magnetic semiconductors "	L. Pereira K.U. Leuven
C5	16:50 – 17:05	"Ion beam nanopatterning of metallic surfaces: A novel mechanism for the pattern formation"	T. Skeren K.U.Leuven, IMEC
C6	17:05 – 17:20	"Two-band superconductors: Hidden criticality deep in the superconducting state"	L. Komendova Univ. Antwerpen

Invited Lecture Condensed Matter and Nanostructure Physics

Graphene as a prototype membrane: Ripples, puddles and strain engineering

Mikhail Katsnelson

(Radboud University Nijmegen, The Netherlands)

Graphene is the first truly two-dimensional crystal (just one atom thick) consisting of identical atoms with the known law of interactions. This makes it a testbed for studying physics and chemistry in two dimensions. Combining atomistic simulations with existing phenomenological theories of fluctuating membranes we can reach much deeper understanding of statistical mechanics of low-dimensional systems in general.

As a result of the general instability with respect to bending fluctuations graphene is rippled, and this effects enormously on its structural, thermodynamic and electronic properties. The latter turn out to be very sensitive to local bending and in-plane deformations. This can be used to modify in a desirable way the electronic structure of graphene with exciting perspectives for electronics (strain engineering).

C1 Contributed Lecture Condensed Matter and Nanostructure Physics

Electronic properties and STM images of N and B doped graphene L.

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Chemical doping of graphene-based materials represents an active research direction to tune their electronic and transport properties in the same way as for conventional doping in semiconductor (Si, ...). Substitution of one (or several) carbon atoms by Boron (B) or Nitrogen (N) atoms give rise to a small structural effect whereas the electronic property is locally modify. Indeed, the substitution by N is expected to show additional donor states and then a n-type doping whereas B substitution lead to p-type doping. This chemical doping also induces changes in the reactivity of carbon nanostructures, thus allowing the development of chemical sensor, energy storage device (Li-battering) or supercapacitor.

Several attempts have been reported in the literature for doping either flat graphene or carbon nanotubes (CNT). STM and STS are key experimental data in order to correlate the production methods and the atomic configuration of modified graphene. They also permit an analysis of the electronic levels in the vicinity of the dopant. Recent simulations [1,5] and experimental achievements [2,3] have shown that N-substitution can be achieved and analyzed.

Another way to tune the electronic properties of graphene material is to modify the number of layer (or the stacking order) of the system. Indeed Multilayer graphene (MLG) presents electronic and transport properties drastically different than single-layer graphene (SLG). The combined influence of both interlayer interaction and of chemical doping has not been investigated in details yet in order to interpret experimental data. In the present study, both Nitrogen and Boron substitutional doping in one of the two layers of a bilayer graphene is investigated using a first-principles approach. A detailed study of the STM features for N or B chemical doping on the top layer of bilayer graphene or for buried defect is performed. Our simulations predict that even if local and direct fingerprints of buried chemical modification are very difficult to image, the delocalisation of the doping charges on the neighboring plane of bilayer graphene leads to a clear modification of the symmetry of the STM patterns, dependent on the bias voltage, for both top-doped and buried-doped layers. Doping multilayer graphene with Bernal (AB) stacking displays hexagonal or triangular STM patterns depending of the sign of the bias and can be misinterpreted as disoriented MLG if a careful STM/STS study is not performed [4].

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Effect of nonhomogenous dielectric background on the plasmon modes in graphene double-layer structures at finite temperatures

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We have calculated the plasmon modes in graphene double layer structures at finite temperatures, taking into account the inhomogeneity of the dielectric background of the system. The effective dielectric function is obtained from the solution of the Poisson equation of a three-layer dielectric medium with graphene sheets located at the interfaces, separating the different materials. Due to the momentum dispersion of the effective dielectric function, the intra- and interlayer bare Coulomb interactions in the graphene double layer system acquires an additional momentum dependence–an effect that is of the order of the interlayer interaction itself. We show that the energies of the in-phase and out-of-phase plasmon modes are determined largely by different values of the spatially dependent effective dielectric function. The effect of the dielectric inhomogeneity increases with temperature, and even at high temperatures the energy shift induced by the dielectric inhomogeneity and temperature itself remains larger than the broadening of the plasmon energy dispersions due to the Landau damping. The obtained new features of the plasmon dispersions can be observed in frictional drag measurements and in inelastic light scattering and electron energy-loss spectroscopies.

Thermal conductivity depth profiling of hardened solids using infrared photothermal radiometry technique based on neural artificial network recognition

Liwang Liu, Jichuan Xiong, Chinhua Wang and Christ Glorieux

The thermal conductivity of materials, very sensitive to heterogeneities, is a quite appropriate thermophysical quantity to probe their microstructure. Laser induced Photothermal radiometry (PTR), based on the generation and detection of thermal waves in the sample being detected, has become a powerful tool for the thermophysical characterization of broad classes of materials, due to its non-destructive and highly sensitive nature. In this paper, we focus on hardened steel samples, in which a depth profile of varying microstructure is induced by a hardening treatment. An artificial neural network recognition approach is used to extract the thermal conductivity depth profile from PTR signals obtained in a non-contact way on flat and cylindrical steel rods. The quality of the reconstructed thermal conductivity depth profile is confirmed by a good correspondence between the signals calculated a posteriori from the profile and the experimental data that were fed to the neural network. The results confirm the expected anti-correlation between the thermal conductivity and the hardness, which was determined from a classical indentation procedure at different depths.
Key words: photothermal radiometry, thermal conductivity, depth profiling, artificial neural network

Lattice location of transition metals in dilute magnetic semiconductors

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The discovery of a dilute magnetic semiconductor (DMS) which is ferromagnetic above room temperature is a critical step towards the development of semiconductor spintronics [1]. For a given impurity-host combination, the magnetic behavior is largely determined by the lattice sites occupied by the magnetic impurities. The canonical example is Mn-doped GaAs (narrow-gap), where Ga-*substitutional* Mn orders ferromagnetically and *interstitial* Mn acts as a compensating defect which reduces the Curie (ordering) temperature. The situation is somewhat different in wide-gap DMS materials such as Co- and Mn-doped ZnO and GaN, for which it is generally accepted that the transition metals occupy only cation substitutional sites.

We present electron emission channeling experiments on the lattice location of implanted Mn and Co in GaAs [2], ZnO [3] and GaN. The technique is based on *channeling* and *blocking* effects acting on the β^- particles emitted during decay of radioactive ^{56}Mn and ^{61}Co impurities implanted at the ISOLDE facility at CERN.

In Mn-implanted GaAs, we show that while the majority of the implanted Mn impurities occupy substitutional Ga sites, up to ~30% occupy tetrahedral interstitial sites with As nearest neighbors. Contrary to the general belief that interstitial Mn is removed by thermal annealing at ~200ºC [4,5], we show that the interstitial fraction persists above 400ºC [2]. We discuss the implications of such high thermal stability of interstitial Mn on the strategies and prospects for achieving higher Curie temperatures in Mn-doped GaAs.

In Co- and Mn-implanted ZnO [3] and GaN, in addition to the expected majority in cation sites, significant fractions (~20%) of the implanted Co and Mn impurities substitute the anion (O in ZnO and N in GaN). We compare these results to previous lattice location studies on ZnO and GaN and discuss how such minority anion-substitution, which had never been considered before, may in fact play an important role in determining the materials' magnetic behavior.

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Ion beam nanopatterning of metallic surfaces: A novel mechanism for the pattern formation

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The irradiation of surfaces with low energy ions often leads to the formation of periodic surface patterns (most typically periodic ripples). This phenomenon has attracted a lot of attention in the last few decades [1,2]. It is a promising nanofabrication technique but at the same time an interesting and complicated physical process. Despite the significant scientific effort, there are still large gaps in the theoretical understanding of the underlying physics.

We focus on the metallic surfaces and in particular we extensively studied the patterning behavior of the Ni(001) surface upon a few keV Ar^+ ion bombardment. We investigated the role of various parameters on the resulting pattern morphology. Based on the experimental data, we developed a novel physical model describing the pattern formation process in our system. The mechanism is based on an interplay between surface defect diffusion and ion erosion, but in contrast to the existing theoretical models, it ascribes the formation of ripples purely to the non-linear erosion dynamics (rather than so-called linear instability). The computer simulations show an excellent agreement with the experiments (Fig. 1). In the context of our model we also discuss the influence of the ion energy and we compare the theoretical predictions with the experimental data.

Moreover, the current model may be important for the overall understanding of the patterning phenomenon in a general system. Our results indicate, that the presently widespread paradigm, that the formation of ripples is a consequence of a linear instability may not always be correct. The non-linear dynamics seems to play a much more prominent role than originally thought.
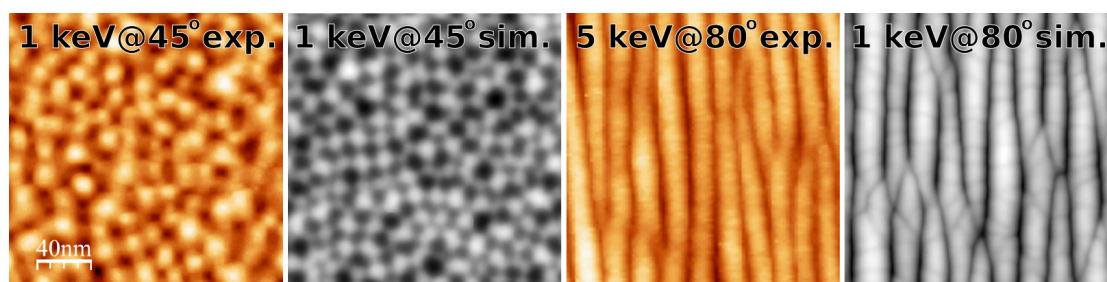

Fig. 1: Mound and ripple patterns created by 1 keV and 5 keV Ar+ ion bombardment (at 45° and 80° angle of incidence respectively, measured from the surface normal), comparison of the experimental and simulated morphologies

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C6 [BP9] Contributed Lecture Condensed Matter and Nanostructure Physics

Two-band superconductors: Hidden criticality deep in the superconducting state

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We found that two-band superconductors harbor hidden criticality deep in the superconducting state, stemming from the critical temperature of the weaker band taken as an independent system [1]. For sufficiently small interband coupling the coherence length of the weaker band exhibits a remarkable deviation from the conventional monotonous increase with temperature, having a pronounced peak close to the hidden critical point. This can strongly affect most of the superconducting properties, and can be experimentally observed (in e.g. multigap borides and pnictides) by imaging of the variations of the vortex core in a broader temperature range. In particular the effects crucially depending on the disparity of the characteristic length scales (e.g. nonmonotonic intervortex interaction [2], appearance of fractional vortices in mesoscopic samples [3]) shall be most pronounced in the vicinity of this hidden criticality.
We will present the analytic proof that the interband coupling is the governing field of this criticality with the same critical exponents as e.g. the magnetic field in the ferromagnetic materials. Furthermore, we will show the numerical results for the evolution of a vortex core with temperature obtained in the microscopic Bogoliubov-de Gennes formalism, which not only proves the existence of hidden criticality, but also motivates further experiments on multiband materials.

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ELASTIC PARAMETERS OF A THIN (300NM) NIMNGA COATING

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Impulsive stimulated scattering(ISS) is an all optical technique that allows to simultaneously investigate the thermal and elastic properties of a material. In the reflection configuration, using a diffraction grating and imaging optics, a pulsed pump laser beam is split into two first orders and recombined at the sample surface thus creating an interference pattern. The energy is delivered in a very short time and the sample thermally expands launching spatially periodic acoustical waves. The dynamically diffracted component of a second CW probe laser beam is used to detect the surface acoustic waves and thermal expansion pattern.
Up to now the technique has been used to investigate, int. al., thin films, multi-layered structures, bulk fluids and fluids at an interface with a solid. In this report the technique is used to investigate a thin layer of NiMnGa on an anisotropic MgO substrate. NiMnGa is a Heusler alloy that has received increased attention because of its magnetic shape memory effect and because of elastic strains of up to 10%. Several authors have reported values for the stiffness parameters of NiMnGa in the austenite phase. In this report we investigate the elastic properties of this material in the, low temperature, martensite phase. The experimental results are analyzed in the framework of a theoretical model for surface acoustic wave propagation in an anisotropic 1D layered medium.

C8 Poster Condensed Matter and Nanostructure Physics

Preparation and characterization of Al-doped zinc-oxide layers: A new transparent electrode material

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We report on the research project on transparent conductive metal oxides, which are used in optoelectronic devices, for example solar cells and flat panel displays. This study focusses on the *in situ* deposition by dc-magnetron sputtering and on the structural characterization of aluminum-doped zinc oxide (AZO) thin layers. XRD is used to determine the structural properties of the sputter target, and of the AZO thin films. Currently, there is a renewed and substantial interest in transparent conductive oxides (TCO's). These materials are of special interest to the industry because of their use in e.g. photovoltaic devices, LCD screens, based on their low resistivity (10^{-4} $\Omega \cdot cm$) and high transmittance for visible light (90%). Indium tin oxide (ITO) is the standard material for all applications demanding a TCO. However limited resources of indium metal make it expensive. Moreover, it has been proven that indium is a toxic material both for the environment and for human beings [1]. Therefore, we report on a promising replacement of ITO, namely aluminum doped zinc oxide. For the *in situ* preparation of the AZO thin films, a homemade sputtering system was used with a base pressure below 10^{-7} hPa. The target has a diameter of 1.5 inch, and is sintered for 1 hour at 900 °C. It consists of ZnO with 1% wt aluminum. The dc-magnetron sputtering was performed with a power of 40Watt. Pre-sputtering was done in an atmosphere of 2.000 hPa Ar pressure. Before starting with the film deposition, 10^{-3} hPa O_2 was added to the chamber. AZO was grown on a (0002) sapphire substrate. The temperature dependence was investigated. The XRD spectra of the AZO thin films proof that growth is preferentially hexagonal and along the c-axis.

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Acknowledgements

The ground state elemental crystals as a guideline for the assessment of solid state DFT accuracy

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A central issue for experimentalists when confronted with property pre- dictions by density functional theory (DFT) is an assessment of the error bars on the computed quantities. These are usually determined by performing calculations for a set of experimentally well-known benchmark systems. For molecules, some commonly accepted test sets are available for the evaluation of various properties at various levels of theory. Similar systematic and broad tests for crystalline solids are not that easily found. There- fore, several basic properties have been computed for a test set with nearly all ground state elemental crystals. This test set contains many different elements, crystal structures and chemical bond types in a natural way. Three general-purpose DFT codes have been employed, using a Perdew-Burke-Ernzerhof functional. The following table summarizes a comparison between VASP and experiment. It presents both the systematic deviation of the DFT numbers and the remaining error bars.

	deviation	error bar
cohesive energy E_{coh} [kJ/mol]	0%	17
equilibrium volume V_0 [A^3/atom]	+4%	0.6
equilibrium bulk modulus B_0 [GPa]	-5%	9
pressure derivative of B_0 [-]	+6%	0.5
elastic moduli C_{ij} [GPa]	-2%	6

Although the major part of the error bars stems from the choice of a particular DFT functional, a sometimes non-negligible part of it is due to the computational approach, and is hence code-dependent. The same test set of elemental crystals can provide insight into this aspect as well. A quality factor Δ has been defined to compare the equations of state for different codes directly. This quantity expresses the rms energy deviation between the E(V) curve of a code under test, and that of the APW+lo code WIEN2k, averaged over the entire test set. WIEN2k is an all-electron method, believed to provide results that are as close as possible to the true results for the chosen functional. For VASP Δ was 1.8 meV/atom, while for GPAW, a similar grid-based code, it was 3.3 meV/atom.

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Characterization and superconducting properties of a superconductor/ferromagnet hybrid system with Co clusters embedded in a Sn matrix

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The superconducting properties of hybrid systems consisting of ferromagnetic clusters randomly distributed in a superconducting Sn matrix were studied. Preformed Co clusters with typical diameters around 2 nm are produced with a laser-vaporization cluster source and have been co- deposited with thermally evaporated Sn on liquid nitrogen cooled SiO2-substrates. Structural characterization of the samples has been done by means of atomic force microscopy and Rutherford backscattering spectrometry. The magnetic and superconducting behaviour of these systems was studied by SQUID magnetometry measurements.

The magnetic behaviour of the Co clusters varies from superparamagnetic to ferromagnetic with increasing amount of embedded Co clusters. The superconducting critical temperature and phase boundary are investigated for different concentrations of Co clusters, ranging from 0 to 30 volume percent.

For the lowest concentration of Co below 20 volume percent, the Co clusters are superparamagnetic. Above 100K, reversible magnetization curves are observed. For higher concentrations of Co, the Co clusters interact with each other and behave as ferromagnetic particles up to 300K. In both regimes, the hybrid systems show superconducting behaviour with a clear increase of the steepness of the phase boundary. For the lowest concentrations of Co, no significant change in TC is observed. The highest concentration of Co did show a decrease of the superconducting critical temperature.

Photofragmentation study of mass-selected binary vanadium-cobalt clusters using time-of-flight spectrometer

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The study of atomic clusters has captured a lot of interest not only because of their intriguing physics but also because of their potential nano-applications. The story is most fascinating since the clusters can be fabricated in a well-defined manner, allowing to manipulate their properties. Doping of clusters is an important method for that purpose since their geometry and electronic shell structure can be modified by varying the size and the composition. In this report, we present the fabrication of bimetallic vanadium-cobalt clusters in a dual-target dual-laser vaporization source coupled to a newly built high-resolution dual-reflectron time-of-flight mass spectrometer. The stability of cobalt-vanadium clusters is studied using photofragmentation. The clusters are then mass-selected by a nanosecond mass gate and subsequently photofragmented by an intense Nd:YAG laser pulse. The information of recorded fragmentation channels allows us to establish better insight into the intrinsic stabilities as well as the geometric structures of those binary clusters.

Single-file diffusion in colloidal systems: the role of hydrodynamic interactions.

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The structural and dynamical properties of pure 1D-interacting colloidal systems are examined by means Brownian Dynamics computer simulations with the inclusion of the hydrodynamic interactions (HI) at the level of the Rotne-Prager Tensor. We analyze homogeneous systems in which we consider two types of direct interaction among colloids, namely, Yukawa and super-paramagnetic. We find that, the HI lead to a correction about ~12% on the time dependence of the mean-square displacement of the single file diffusion which known to be $t^{1/2}$. Also, we analyze systems where a sinusoidal external field is applied and we focus our attention on the commensurability effects on the dynamics of the system. We find that the correction on the time dependence of the mean-square displacement is enhanced due to the coupling among the external-field, direct -interactions and the HI. Specially for the commensurability $p=1$, our findings are that the systems go from a sub-diffusive to a supper-diffusive behavior and the mobility factor decays exponentially according with the increment on the intensity of the external field.

C13 [BP15] Poster Condensed Matter and Nanostructure Physics

Superconducting proximity effect with Pb nanoparticles embedded in an Al matrix

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We investigate the superconducting properties of Pb nanoparticles (with a diameter varying between 8 and 20 nm) synthesized by ion implantation and subsequent annealing in an Al matrix. The critical temperature T_c of those new types of superconductors is found to increase linearly with the Pb/Al volume ratio. The experimental data is in excellent agreement with the theoretical predictions of the proximity effect in the Cooper limit for strongly coupled superconductors. The remarkably good agreement between theory and experiment implies that the quality of the interface between the nanoparticles and the Al matrix is very good (high transparency). Furthermore, the critical fields and critical currents of those hybrid superconductors have characterized extensively to obtain their full phase diagrams and analyze in detail their physical properties.

Understanding binary and ternary silicide solid phase reactions using complementary *in situ* real-time techniques

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Silicides have been used as electrical contact material in silicon CMOS technology for several decades. A silicide is a compound between a metal atom and silicon which is thermally grown in a solid phase reaction (SPR). Driven by the ever shrinking scale of devices, industry has consecutively shifted from the binary silicides $TiSi_2$, $CoSi_2$ and NiSi to the ternary silicide $Ni_xPt_{1-x}Si$. The addition of a well-chosen ternary element such as Pt, is necessary to make the contact morphologically and thermodynamically more stable. Whereas binary systems such as Ti-Si, Co-Si and Ni-Si have been extensively studied and are more or less understood, ternary silicide systems are far more complex, as their behavior cannot be explained by simply taking the sum of two binary systems. Additives will redistribute during the solid phase reaction (SPR) and can therefore influence the phase formation sequence, kinetics and texture development, depending on their location in the silicide film.

To this end *in situ* real-time techniques are extremely valuable in gaining a profound insight in the involvement of alloying elements during the SPR. In a real-time measurement the specimen is studied throughout the thermal treatment to scrutinize different physical properties continuously as a function of temperature in a single run. This largely reduces the risk of overlooking transient but important steps during the thermal treatment. Also, small but important differences due to sample preparation and thermal treatment can be prevented and the amount of specimens that need to be prepared can be greatly reduced, strongly enhancing the time efficiency.

X-ray diffraction (XRD) and Rutherford backscattering spectrometry (RBS) are techniques widely used in materials research and can both be applied in real time yielding complementary information on the silicide reaction. Information about the crystalline phase formation, phase sequence, formation temperatures, missing phases and texture is readily accessible via *in situ* X-ray diffraction (XRD). However, to fully understand the influence of alloying elements on the phase formation, it is essential to understand the diffusion kinetics and to know where the elements reside during the SPR. For this, *in situ* RBS is the technique of choice. The kinetic parameters, as well as the redistribution of the different elements can be probed as a function of temperature. The complementary information obtained when the results from *in situ* RBS are combined with the result on crystalline phase formation obtained by *in situ* XRD enables one to fully understand the silicide reaction and to disentangle the influence of the alloying element on the silicide formation properties.

In this poster the power of utilizing both complementary *in situ* real-time techniques, i.e. *in situ* RBS and *in situ* XRD, will be demonstrated, presenting examples mainly focusing on silicide solid phase reactions.

Ordered gold and FePt nanoparticle arrays created by the micellar method

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Ordered nanoparticle arrays are of great interest both from the point of fundamental physics as well as of the applied physics. One of the examples to the latter is the field of patterned magnetic storage media. [1] On the other hand nanoparticle superlattices (ordered nanoparticle arrays) can also be of fundamental scientific interest when the particles are embedded in matrices with different electronic properties. The interface-effects between the nanoparticles and the surrounding matrix, also the interparticle-interactions mediated or screened by the matrix, where periodicity can play an important role indeed can have fundamental effects on the electrical properties in macroscopic scales.

As a first example normal metallic nanoparticles embedded in a superconducting matrix act like weak spots where the magnetic flux-quanta can penetrate the superconducting matrix. Macroscopic phenomena raised by the commensurability of the nanoparticle superlattice and the vortex-lattice (Abrikosov-lattice) could be expected. As a second example when the particles are superconducting and the matrix is in normal metallic phase the superconducting current penetrates into the normal phase. If the particles are smaller than the superconducting coherence length the particles can interact with each other like a periodic multi-SNS junction, thus global superconductivity can be achieved. The third example is when the particles are magnetic and the matrix is superconducting. As we know superconductivity and magnetism are fundamentally excluding each other, magnetic field breaks down superconductivity (via magnetic pair breaking effect) and vica versa, superconducting current screens the magnetic field penetrating into it (Meissner-effect). In the presence of an exchange field spatially oscillating superconducting order parameter has been predicted and observed, even predictions were made of the enhancement of superconductivity.

In our work we present an emerging bottom-up method to produce ordered nanoparticle arrays of metallic, superconducting and magnetic materials with controllable nanoparticle sizes and spacings using the micellar method for the investigation of the proximity effects in the above described three type of embedded nanoparticle systems. We use atomic force microscopy (AFM) to characterize the assemblies concerning angular correlation, size and spacing distributions. We show that with gold nanoparticles good hexagonal ordering and narrow size distribution can be achieved. We also synthesized FePt nanoparticle arrays only with less pronounced angular correlation and wider size distribution compared to the gold sample.

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C16 [BP16] Poster Condensed Matter and Nanostructure Physics

Changing magnetic properties of nanocluster assembled films using hydrogen

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Using preformed gas phase Co nanoclusters and subsequent deposition thin nanogranular films were produced. These films were characterized using magnetic force microscopy and vibrating sample magnetometry. Tailoring of the magnetic properties in these nanocluster assembled films was achieved by admitting a small percentage of H_2 gas (~2%) into the Co gas phase formation chamber prior to deposition. The oxygen content in the films is considerably reduced by the presence of hydrogen during the cluster formation [1], leading to enhancement of magnetic interactions between clusters. This hydrogen-passivation method can be used to tailor the oxidation level thus controlling the magnetic properties of ferromagnetic cluster-assembled films. Further a method was tested to estimate the exchange field and the exchange constant in the samples. This model is originating from the random anisotropy model. For nanocluster assembled thin films an experimental formula for 3 dimensions was taken from reference [2]. Our results are in agreement with this experimental formulation in the case of the sample produced with H_2 gas.

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Reactivity of bimetallic gold clusters

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Gold is a noble metal, but when its size is reduced to the nanometer scale, it loses its nobleness and becomes reactive. We present an extended experimental study on the reactivity of medium sized bimetallic gold nanoclusters. The clusters are produced in a laser vaporization source and subsequently pass through a low-pressure collision cell containing a reactive gas. The abundances of reacted and non-reacted clusters are measured with time-of-flight mass spectrometry as function of the reactant gas pressure. The overall process is considered as a two-step process:

$$\mathrm{Au}_n M^{0,+} + \mathrm{CO} \underset{k_\mathrm{D}}{\overset{k_\mathrm{f}}{\rightleftharpoons}} \mathrm{Au}_n M\mathrm{CO}^{0,+} \xrightarrow{k_\mathrm{D}} \mathrm{Au}_n M^{0,+} + \mathrm{CO}$$

$$\underbrace{\hphantom{\mathrm{Au}_n M^{0,+} + \mathrm{CO}}}_{\text{Inside reaction cell}} \quad \underbrace{\hphantom{\mathrm{Au}_n M\mathrm{CO}^{0,+}}}_{\text{Outside reaction cell}}$$
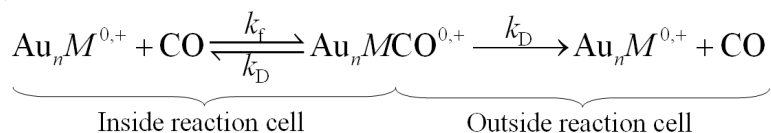
The association rate constant k_f is derived using hard-sphere collision theory and the dissociation rate constant k_D is then derived by fitting the data. Comparing the result obtained by the LPCC technique with that of the ICR technique from Kappes's[1] group for cationic gold clusters at room temperature confirms the applicability of the LPCC technique in studying the cluster's reactivity.

The reactivity of the bimetallic gold clusters is examined as function of size, dopant, charge state, reactant gas and temperature. First, the CO adsorption of neutral, doped gold clusters ($\mathrm{Au}_n M$; M = V, Y, Ag; n=10-30) is compared with that of neutral bare gold clusters.[2-4] Strong size dependences are observed for all dopant atoms, which partially can be related to electronic shell closings. However, the odd-even staggering, which is present for bare and Ag doped gold clusters, diminishes for Y and V doped gold clusters. Next, the CO reactivity of neutral and cationic V doped gold clusters ($\mathrm{Au}_n V_m$; n=10-30; m=1-3) are compared. An enhancement of the reactivity for cationic clusters is observed, which is due to the more facile s-donation from CO towards cationic clusters. Last, the effect of the cluster temperature on the cluster reactivity is examined. There is a clear decrease of the reactivity with the increase of the cluster's temperature, which is due to the activated backward reaction.

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First-principles Study of Metal Adatom Adsorption on Silicene

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Motivated by the very recent experimental advances on the synthesis of monolayer silicone sheets, in this study we investigate the adsorption of alkali metal, alkaline earth metal and *3d*-transition metal adatoms on silicene by using first-principles density-functional theory. Most favorable adsorption site, binding energy, magnetic ground state, energy band spectrum, dipole moments, electronic charge transfer and work function of the adatom-silicene system are calculated. Our calculations show that adsorption characteristics of silicene are quite different than graphene. For alkali metals and alkaline earth metals, as a result of large charge transfer from adatom to silicene adatom+silicene structure becomes metallic. Upon adsorption of these materials work function of the silicene sheet is lowered. It is calculated that the larger atomic radius, the larger decrease in work function. However, upon the adsorption of *3d*-transition metal adatoms, depending on the adsorbate, structure can become semiconductor, half-metal or metallic states. Adsorption of almost all metal adatoms, except Zn, can be characterized by covalent bonding between adatom and silicene. While structure remains nonmagnetic upon the adsorption of alkali and alkaline earth metals, *3d*-transition metal atoms are likely to make silicene sheet magnetic. Our calculations reveal that silicene is superior to graphene due to its diverse adsorption properties.

Band gap engineering in InAs/GaSb core-shell nanowires

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Broken bandgap heterostructures made from the lattice matched semiconductors InAs and GaSb have gathered a lot of attention in recent times, from using them as infra-red lasers and detectors[1–3] to the prediction of topological insulating[4] behaviour. Because the valence band maximum of GaSb is above the conduction band minimum of InAs, charge separation may occur in which electron states localize in InAs and holes in GaSb. The effect of confinement on this band structure can now be tuned[5–7] by changing the size of either InAs or GaSb regions in the heterostructure. We have studied the band structure for InAs/GaSb core-shell nanowires using the 8 band k.p method[8,9]. It is observed that the hybridization[10] of conduction and valence band states can be achieved by varying the radius of the InAs/GaSb nanowire as well as the radius of the core part. This hybridization leads to semi-metallic[11] character to the otherwise semiconductor structures. Apart from the negative effective bandgap in the semi-metallic case, also a minigap[12,13] can appear in certain structures away from the zone center. This minigap is responsible for a reduction of the conductivity in the semi-metallic regime. We have studied both this negative effective bandgap and the minigap of InAs/GaSb core-shell nanowires by varying the size of both InAs and GaSb regions.

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Vibrational properties of nanographene

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The eigenmodes and the vibrational density of states of the ground state configuration of graphene clusters are calculated using atomistic simulations. The modified Brenner potential is used to describe the carbon and hydrogen inter-atomic interaction. For a given configuration of the C-atoms in nano-graphene the eigenvectors and eigenfrequencies of the normal modes are obtained after diagonalisation of the dynamical matrix whose elements are the second derivative of the potential energy. The compressional and shear properties are investigated from the divergence and rotor of the velocity field. For symmetric clusters and defective clusters with pentagon arrangement on the edge, the highest frequency modes are shear modes. The constant-volume specific heat of the clusters is also calculated within the harmonic approximation and the convergence to the result for bulk graphene is investigated.

Ginzburg-Landau theory of the Linear-zigzag structural transition in quasi-one-dimensional classical Wigner crystals

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We present a study of the structural zigzag phase transition in a quasi-one-dimensional confined system of strongly interacting particles. The particles are assumed to interact through a screened power-law potential ($r^{-n}e^{-\lambda r}$) and the confinement potential is taken of a general power-law-type ($|y|^{\alpha}$). With increasing density or decreasing confinement the ordered particles undergo a zigzag transition, i.e. the system makes a continuous transition from a single chain to a double chain configuration. We develop a mean-field description of this zigzag phase transition. The parameters of the resulting one-dimensional Ginzburg-Landau theory are determined analytically for different values of α and n. Close to the transition point for the zigzag phase transition, the scaling behavior of the order parameter is determined. For $\alpha = 2$, we generalized our approach to the case of two vertically coupled quasi-one-dimensional channels.

Nanostructured thin films for Solid Oxide Fuel Cells: crystallographic properties
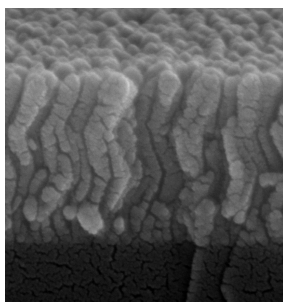
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A fuel cell converts the chemical energy from a fuel into electricity through a chemical reaction. The fuel is oxidized at the anode, while oxygen reacts on the cathode. The cathode and anode are separated by an electrolyte. In Solid Oxide Fuel Cells (SOFC) the electrolyte is an oxygen ion conductor such as Yttria Stabilized Zirconia (YSZ). To lower the process temperature of the SOFC the film thickness of the electrolyte must be reduced. The bulk properties of these materials are well known but when down scaled to a thin film the fundamental aspects of the oxygen ion conduction change due to the occurrence of small scale or nano-effects. That is why, a good understanding of the microstructure and crystallinity would open the possibility to manipulate the ionic conductivity by controlling the nanocrystalline microstructure of the thin film.

With dual magnetron sputter deposition, thin films of solid state electrolytes can be grown. This technique allows the deposition of thin films ranging in thickness from a few nanometers to micrometers and to investigate the compositional influence in a flexible way.

In this study the experimental conditions were varied to modify the microstructure and texture of the YSZ thin films. Especially the pressure, and the source-substrate distance showed an interesting influence on the thin film properties. From crystallographic point of view the films show the interesting feature of biaxial alignment. The crystals have a preferential out-of-plane and in-plane alignment, meaning that for a low misorientation angle, between the adjacent grains, the crystallographic properties of the polycrystalline thin film are comparable to a single crystal thin film. The films are built from well-defined V-shaped facetted columns. The constituent columns are tilted towards the zirconium source. This behavior has been investigated in more detail, and can be tuned by changing the geometrical configuration of the deposition set-up. As a result, zig-zag nanostructured columns can be grown.

Spectroscopy visualization of acoustic clapping with photorefractive interferometry

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Nonlinear acoustic methods have demonstrated high potential in recent years in the field of nondestructive testing (NDT) due to their enhanced sensitivity and especially their "defect selective" behavior. Many defects in materials involve non-bonded surfaces which causes contact acoustic non-linearity (CAN). Higher harmonics of the frequency of the driving harmonic vibration can be generated through two mechanisms; energy dissipation due to the tangential friction of the boundaries and "mechanical rectification" due to interface clapping. Several full-field imaging techniques have been implemented to exploit the potential of this effect, including shearography [1] and scanning laser Doppler vibrometry [2]. While shearography is subject to a complex relation between the interferograms and the acoustic displacement, namely non-straightforward interpretation of the results, scanning laser Doppler vibrometer needs to compromise between optimum spatial resolution and speed of operation. In this paper, a photorefractive interferometry method [3] is elaborated to visualize nonlinear acoustic phenomenona while overcoming the disadvantages in the above mentioned techniques. As a proof of concept, a PVDF film is harmonically excited, with a metal tip touching its surface, which creates the "mechanical rectification" and higher harmonics of the excitation frequency arise at the location of the clapping. By utilizing the narrow-band feature of the photorefractive crystal, and mixing down the frequency of vibration patterns by choosing a proper phase-modulation frequency of the reference beam of the interferometer, vibration components of interest, e.g. higher harmonics due to "mechanical rectification", can be selectively imaged, while disturbing optical effects due to the strong vibration component of the excitation frequency are suppressed. This results in outstanding performance on detection of acoustic nonlinearity in the presence of strong background linear acoustic motions. Acoustic nonlinearity can be imaged without scanning by providing a full-field interferogram with the intensity of each pixel directly proportional to the displacement amplitude at the corresponding point on the sample surface. Absolute measurement of the surface dynamics can be performed with micrometer resolution in the imaging plane and in depth.

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C24 Poster Condensed Matter and Nanostructure Physics

Effect of film thickness on the optical behavior of silver nanoparticles/polymer nanocomposite films∗

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Dispersion and chemical stability of nano-objects in a dielectric matrix remains a challenge in nanocom- posite films preparation. For noble metal nanoparticles (NPs) (Ag, Au . . .), in situ synthesis methods exist : the chemical reduction of a noble metal salt is achieved either by thermal annealing or by photore- duction and the polymer matrix acts as a reducing agent. These "one-pot synthesis" protocols are usually simpler than ex situ synthesis methods but their mechanism is today not fully understood although being the subject of an increasing number of publications. Since the pioneering work of Oates and coworkers[1], the optical properties of silver NPs/polymer films can be efficiently probed by spectroscopic ellipsometry (SE). They are characterized by the presence of an strong absorption peak due to the surface plasmon- polariton resonance (SPPR) phenomenon[2]. In recent articles[3,4], we studied, using AFM analysis and SE, that the effect of the annealing time on the onset of the plasmon resonance in thick films (d > 500 nm). In this paper, we considered the optical behavior of thin (20nm) and thick (300nm) Ag-doped polymer films at high silver content. The topography of the films was studied by atomic force microscopy and the roughness parameters of the thin films were found to be larger than those of the thicker ones. The parameters of the surface plasmon-polariton resonance are also thickness-dependent (Fig. 1).
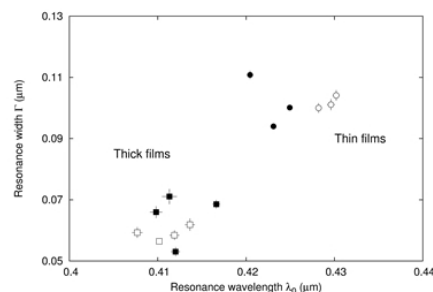

Figure 1: Resonance width(Γ) versus resonance wavelength (λ_0) for Ag-PVA films (open symbols : 12%Ag;plainsymbols: 2.5% Ag)

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Imaging ellipsometry of thermochromic materials : optical properties at the (sub)-micron scale∗

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VO2 is a material which undergoes a reversible crystal-structural phase transition from monoclinic to tetragonal (rutile type) at 68 ∘C. This phase transition is accompanied by strong variations in conductivity, in magnetic as well as in optical properties. For this reason, VO2 is known as a thermochromic material and has been proposed as a 'smart' coating for windows with variable solar gains adapting to the ambient temperature. Recently, for the first time, thermochromic films of VO2 were successfully deposited by DC reactive magnetron sputtering on atypical stainless steel substrate1 and their optical properties analyzed using spectroscopic ellipsometry (SE). The drawback of the technique is that the optical and structural parameters are averaged over the spot size. For smooth and homogeneous samples, this drawback has no consequence but for anisotropic or polycrystalline materials (Fig. 1) the consequences can be important, leading to averaged (and rather incorrect) optical properties. One possibility to access to the local optical properties at the (sub-)micron scale is to consider imaging ellipsometry (IE), a technique which yields images of the ellipsometric parameters (Ψ and Δ maps). Multivariate statistical strategies have been proposed to considerably reduce the time devoted to the data analysis2.

In this paper, we used IE to show the complex evolution of the optical properties of VO2 samples on stainless steel substrate as a function of the temperature. Ellipsometric images sequences reveal the complexity of the thermochromic transition.
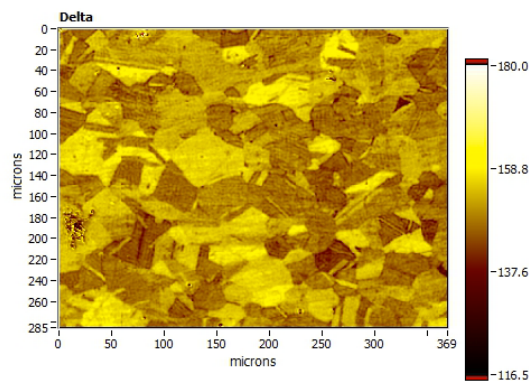
Figure 1: Imaging ellipsometry Δ map : 100nm-thick VO2 film on stainless steel substrate (Magnif. : 10 ×)

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Aharanov-Bohm oscillations revealed through the vortex dynamics in superconducting hollow cylinders

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Using time-dependent Ginzburg-Landau theory we demonstrate that the Aharanov-Bohm effect, resulting from a Berry phase shift of the (macroscopic) wave function, can be revealed through the dynamics of topological phase defects present in that same wave function. In particular, we study vortices and antivortices on the surface of a hollow superconducting cylinder, moving on circular orbits tracing out the cylinder cross-section as they are subjected to the force from the current flowing parallel to the cylinder axis. These orbits get deflected by the presence of a magnetic field component along the cylinder axis. The orbit deflections become periodic as a function of magnetic field, varying between minimal circular orbits and elongated ellipsoidal orbits, swivelling back and forth due to the Aharanov-Bohm effect. This leads to strong and robust resistance oscillations between the extremities of the cylinder. The oscillations are in antiphase with the Little-Parks oscillations and they are observable in a broad range of relevant parameters, e.g., much below the critical temperature. The detailed shape of the oscillations demonstrates hysteretic effects, related to topological pinning of vortices on a curvilinear cylindrical shell.

Microscopic mechanisms for the Fermi-liquid response of Nb-doped strontium titanate

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The experimentally detected Fermi-liquid behavior of the DC resistivity for the Nb-doped strontium titanate [1] is theoretically investigated involving different scattering channels. It has been established that the total relaxation rate in $SrTi_{1-x}Nb_xO_3$ is provided by two mechanisms. First, the Baber electron-electron scattering [2] with participation of both Coulomb and phonon-mediated electron-electron interactions provides the T^2-dependence of the resistivity and of the relaxation rate. Second, the scattering on the potential landscape caused by impurities is responsible for the residual relaxation rate which does not vanish at $T = 0$. The calculated relaxation rates are in agreement with the experiment [1]. The aforesaid agreement can be achieved only accounting for all phonon branches in $SrTi_{1-x}Nb_xO_3$ including the acoustic phonons. It is remarkable that the resulting effective electron-electron attraction can overcome the Coulomb repulsion in strontium titanate. Thus the superconductivity and the Fermi-liquid properties of Nb-doped strontium titanate have the common origin, as suggested in [1].

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Action spectroscopy to investigate the optical absorption spectra of small gold-palladium cluster cations

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We used the action spectroscopy technique that combines wavelength dependent Xe messenger atom photodetachment and mass spectrometry to investigate the electronic excitation spectra of Au and bimetallic Au-Pd cluster cations. The optical absorption spectra of pure Au_n and Pd doped $Au_{n-1}Pd$ cluster cations ($16 \leq n \leq 20$) were measured in the gas phase by use of the corresponding cluster-Xe complexes in the photon energy range of $1.8 - 5$ eV. The influence of the Pd dopant atom on the optical spectra of the Au_n clusters, which form hollow cages (n = 16-18) [1] and a highly stable tetrahedron (n = 20) [2] is discussed. In addition, the geometry change for the larger cluster sizes (Au_n and $Au_{n-1}Pd$, n > 20) is clearly demonstrated via their ability to attach Xe atoms. Analogical change in the cluster ability to attach Ar atoms was readily observed at 2D-3D transition of pure Au clusters.

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Structural trends and band gaps within the Al-Zn-O system

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In an age of flat screens and solar panels, a decent and affordable transparent conducting oxide (TCO) is essential. Tin-doped indium-oxide (ITO) meets the technical demands, but is economically less attractive due to the scarcity of indium. A possible alternative is Aluminum- doped zinc-oxide (AZO), though its conductivity does not yet reach that of ITO. A better understanding of how the aluminum influences ZnO is necessary.

In this work, we have applied various structure prediction tools to the Al-Zn-O system. For a set of given stoichiometries, several crystal structures were determined that are either the ground state for that stoichiometry or close to the ground state. Although these materials do not appear in nature themselves, they serve as virtual experiments to observe how Al behaves in a ZnO matrix, at various concentrations. Extrapolation of the observed trends to the regime of low Al-concentrations provides new insight that is relevant for understanding AZO.

Next to structural information also the band gaps have been monitored over this set of metastable crystals, using both the PBE functional and the modified Becke-Johnson functional. Trends for both sets of bandgaps will be discussed.

Keywords: Transparent Conductive Oxides, AZO, structure prediction, band gaps.

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Localized state and charge transfer in nitrogen-doped epitaxial grapheme

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Nitrogen-doped epitaxial graphene grown on SiC(000-1) was prepared by exposing the surface to an atomic nitrogen flux. The atomic nitrogen was produced by a remote RF plasma source. The exposure results in the creation of nitrogen-related defect sites in the graphene lattice, the concentration of which depends on the exposure time (the settings of the plasma are held constants for each sample).

Using Scanning Tunneling Microscopy (STM) and Spectroscopy (STS), supported by Density Functional Theory (DFT) calculations, the simple substitution of carbon by nitrogen atoms has been identified as the most common doping configuration, as in ref. [1] (although the production method is different). High resolution images reveal a reduction of local charge density on top of the nitrogen atoms, indicating a charge transfer to the neighboring carbon atoms. For the first time, local STS spectra clearly evidenced the energy levels associated with the chemical doping by nitrogen, localized in the conduction band. To highlight this state, the tunneling spectra above the defect and above the graphene have been taken at constant tip's height. This allowed to unambiguously identify the donor-state of the substitutional nitrogen.

The shift of the Dirac point and the n-doping level associated have been estimated, giving a charge transfer of 0.8 electron by dopant atom. However, STS should be completed by a complementary technique (as ARPES) to confirm this point as it is known that the tunneling spectra of graphene around the Fermi level are perturbed by the absence of a phonon-induced channel (ref [2]).

Various other nitrogen-related defects have been observed. The bias dependence of their topographic signatures demonstrates the presence of structural configurations more complex than substitution as well as hole-doping. Additional work is being carried out to acquire the STS signature of those more complex defects in order to identify them confidently.

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Quasicondensation and pseudogap in two-dimensional Fermi gases

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Within the Gaussian pair fluctuation formalism, which is an improvement of Nozières – Schmitt-Rink approach, the phase diagrams for imbalanced Fermi gas with *s*-wave pairing are obtained accounting for both phase and amplitude fluctuations. A special attention is paid to the pseudogap paired state above the Berezinskii-Kosterlitz-Thouhless transition temperature. The amplitude of the order parameter is other than zero in the pseudogap state, while the phase coherence is absent. The Gaussian pair fluctuation approach yields a convergent fermion density for the paired state in 2D. Owing to the fluctuations, the pairing temperature for the pseudogap state can be substantially lowered with respect to the mean-field critical temperature. This difference is especially drastic in the strong-coupling regime. The obtained pairing temperatures are in agreement with recent experimental data on pseudogap pairing of ultracold fermionic atoms in two dimensions. The obtained results can shed light on the pseudogap state for high-temperature superconductors.

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Magnetic reorientation of nanoscale magnetic islands due to close proximity with a superconducting film

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The interplay between magnetism and superconductivity is an important research field both from theoretical and experimental point of view. These hybrid systems show remarkable variations of their superconducting as well as magnetic behavior, e.g. proximity-induced magnetism [1], vortex pinning [2], ratchet motion [3] etc. However, in most cases the magnetic material does not undergo major changes upon going through the superconducting phase transition, despite the fact that they mutually interact. In proper conditions, i.e. when the energy for magnetic ordering and pairing energy of the superconductor are comparable, the superconductor should become strong enough to influence the properties of the magnetic material significantly [4].

In order to reach this regime, small nano-islands of ^{57}Fe with different sizes (1-10 nm) were grown on a MgO(100) substrate and covered by a 60 nm Nb thin film. Nuclear resonant scattering (NRS) provides a unique tool to investigate the magnetic and chemical environment of the ferromagnetic nano-islands when the superconducting overlayer is above or below its superconducting critical boundary [5]. The hyperfine parameters of the Fe are investigated as a function of temperature and external magnetic field while the resistance of the sample is monitored in situ via four probe measurements. Besides a peculiar magnetic susceptibility of the Fe islands, a clear influence of the superconductor is visible in the NRS spectra (Fig. 1). For example, the thin superconducting layer forces the island macrospins in particular directions. Low-energy muon spin rotation measurements complement the NRS measurements by providing local information on the field distribution inside the superconducting layer [6]. The combination of both techniques provides us a unique tool to obtain a deeper insight in the mechanisms used by the bilayer system to minimize its energy.

Fig. 1: A. Selection of spectra at different temperatures in a zero external magnetic field. B. Extracted out-of-plane angle as a function of external applied field above, below and close to the superconducting phase boundary.

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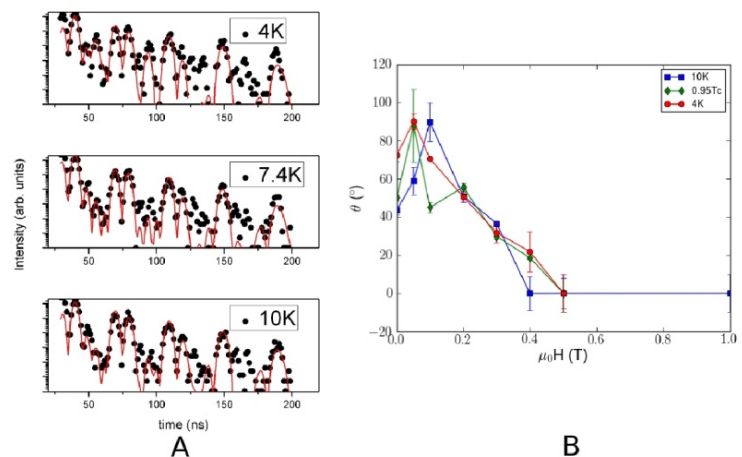
Evolution of the phonon density of states of Nb_3Sn in thin superconducting films: experiment and theory

S. Couet[1], H. Peelaers[2], M. Trekels[1], C. Petermann[1], M. Van Bael[3], A. Vantomme[1], B. Partoens[2], F.M. Peeters[2], K. Temst[1]

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Atomic vibrations in solids, i.e. phonons, determine macroscopic properties like heat capacity. Phonons also play a central role in cooperative phenomena such as superconductivity, were electron-phonon coupling properties determine superconducting parameters. In nanoscale objects such as thin films, it is know that the phonon density of state (PDOS) can be modified compared to bulk. In the case of superconductor, a modification of the PDOS will directly influence the electron-phonon coupling and hence, the superconducting properties.

Here we present a joint experimental and theoretical effort aiming at resolving the phonon density of states of Nb_3Sn thin films. Experimentally, it is very challenging to measure the phonon density of state of thin films. For that purpose, we use the isotope sensitive technique of nuclear inelastic scattering (NIS) applied on the ^{119}Sn resonance and measure the partial density of state of Nb_3Sn thin films of different thicknesses. These results are compared with ab-initio calculations. A good match of the experimental and theoretical PDOS allows us to use the data to calculate the phonon contributions to the decrease of the T_c in Nb_3Sn films.

PARALLEL SESSION (D)

PARTICLE AND NUCLEAR PHYSICS

Auditorium E.0.12, 15:00 – 17:30

Chairman: Michael Tytgat (Universiteit of Ghent)

Invited lecture:

15:00 – 15:40   "Exploring the final frontier"   N. Van Eijndhoven
                                                                                V.U.Brussel

Contributed Lectures:

D1   15:40 – 15:55   "The Askar'yan Radio Array"   Th. Meures
                                                                        U.L.Bruxelles

D2   15:55 – 16:10   "The ratio method to study exotic nuclear   P. Capel
                        structures"   U.L.Bruxelles

D3   16:10 – 16:25   "Yet Another way to hide Lambda"   A. Koshelev
                                                                        V.U.Brussel

D4   16:25 – 16:45   "Supersymmetry searches at CMS"   A. Kalogeropoulos
                                                                        V.U.Brussel

D5   16:45 – 17:00   "Collider signatures of goldstini in gauge   K. De Causmaecker
                        mediation"   V.U.Brussel

D6   17:00 – 17:15   "Gravitino production at LHC"   B. Oexl
                                                                        V.U.Brussel

IceCube : Exploring the final frontier

Nick van Eijndhoven

Vrije Universiteit Brussel – IIHE (ULB-VUB)

Astroparticle Physics revolves around phenomena that involve (astro)physics under the most extreme conditions. Cosmic explosions, involving black holes with masses a billion times greater than the mass of the Sun, accelerate particles to velocities close to the speed of light and display a variety of relativistic effects. The produced high-energy particles may be detected on Earth and as such can provide us insight in the physical processes underlying these cataclysmic events. Having no electrical charge and interacting only weakly with matter, neutrinos are special astronomical messengers. Only they can carry information from violent cosmological events at the edge of the observable universe directly towards the Earth.

At the Inter-university Institute for High Energies (IIHE) in Brussels we are involved in a world wide effort to search for high-energy neutrinos originating from cosmic phenomena. For this we use the IceCube neutrino observatory at the South Pole, the world's largest neutrino telescope which has been completed (including its DeepCore extension) in december 2010 and is currently taking data.

One of the research areas at the IIHE comprises studies of transient phenomena, i.e. Gamma Ray Bursts (GRBs) and flares of Active Galactic Nuclei (AGN), which are believed to be the most violent cosmic explosions involving black holes and neutron stars.

In this talk I will present the underlying ideas of high-energy neutrino production in explosive cosmic phenomena and the IceCube detection principles. It will be shown how the combination of IceCube data with satellite observations opens up the possibility of identifying high-energy neutrinos originating from transient cosmic events for the first time in history. Also the potential of Dark Matter searches with IceCube will be addressed and some recent general experimental results will be presented.

D1 Contributed Lecture Particle and Nuclear Physics

The Askar'yan Radio Array

Thomas Meures, Kael Hanson, Yifan Yang

Université Libre de Bruxelles – IIHE (ULB-VUB)

At South Pole, the construction phase of the ultra-high energy (UHE) neutrino detector ARA (Askaryan Radio Array) has been started. In winter season 2011-2012, next to the previously installed prototype, the first ARA station has been deployed and is taking data since then. By 2016, 36 more stations will be installed, each consisting of 16 antennas situated 200m below the ice surface. These stations, covering an area of about 200km^2, form the full ARA observatory, which will be the most sensitive detector for UHE neutrinos. By utilizing the Askaryan effect, emission of radio waves by neutrino induced cascades in the ice, ARA will be sensitive to cosmic neutrinos in the energy range between 0.1 and 10 EeV.

This presentation will give insights into ice properties obtained from real data taken with the prototype station. Moreover it will give a short introduction into smart firmware-based trigger developments, based on simulations of signal propagation from the cascade through the ice to an ARA station. These filters must pick signal from noise based on antenna hit time patterns. Since digitization and readout capabilities are limited, the goal of these filters is to reduce the trigger rate of the actual antenna triggers by a factor of 10^4, which will significantly enhance the sensitivity of the detector as it permits the antenna thresholds to run close to the thermal noise floor.

The ratio method to study exotic nuclear structures

Pierre Capel

Université Libre de Bruxelles

The advent of radioactive-ion beams in the 80s has enabled nuclear physicists to study nuclei far from stability. Exotic structures have been discovered thanks to this technical breakthrough, including halo nuclei. These neutron-rich nuclei exhibit a large matter radius, which is explained qualitatively by their small binding energy of one or two neutrons in a partial wave with low orbital angular momentum. These valence neutrons can thus tunnel far away from the other nucleons and form a sort of diffuse halo around the core of the nucleus. The study of halo nuclei, is usually performed through indirect techniques, such as reactions. Unfortunately, the complexity of the reaction mechanism and the uncertainty in the choice of projectile-target interactions can cause ambiguities in the analysis of measurements. We present here a new way to extract information about the structure of halo nuclei through reactions [1]. The basic idea of this new technique is to study the ratio of angular distributions for breakup and scattering. These two processes exhibit very similar features that depend mostly on the projectile-target interaction [2]. The recoil excitation and breakup model [3] predicts that their ratio gives access to halo-structure information by removing the major dependence on the reaction mechanism and the projectile-target interaction. We check this within the dynamical eikonal approximation [4] and show that the ratio clearly reveals projectile-structure information such as the binding energy and orbital of the halo neutron. Experimentally, the ratio has the advantage not to depend on the absolute normalisation of the cross sections.

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[2] P. Capel, M. Hussein, and D. Baye, Phys. Lett. B 693, 448 (2010)
[3] R. Johnson, J. Al-Khalili, and J. Tostevin, Phys. Rev. Lett. 79, 2771 (1997)
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Yet another way to hide Λ

A. Koshelev

Vrije Universiteit Brussel

I shall show how it is possible to replace the cosmological constant with a somewhat more physical term inspired by non-local models and shall discuss consequences and limitations of this particular approach.

D4 Contributed Lecture Particle and Nuclear Physics

Supersymmetry searches at CMS

Alexis Kalogeropoulos

Vrije Universiteit Brussel – IIHE (ULB-VUB)

We present an overview of current searches for Supersymmetry produced in p-p collisions at the LHC, operating at sqrt(s) = 7 TeV from CMS collaboration. We consider final states with large hadronic energy and missing energy, including also those with isolated photons or leptons, or with topologies signifying long-lived particles that decay in the detector.

D5 Contributed Lecture Particle and Nuclear Physics

Collider signatures of goldstini in gauge mediation

K. De Causmaecker

Vrije Universiteit Brussel – IIHE (ULB-VUB)

I will discuss the collider signatures of the multiple goldstini scenario in the framework of gauge mediation. These models have a visible sector (like e.g. the MSSM) that is coupled by gauge interactions to more than one SUSY breaking sector. The nature of the collider signatures is mostly determined by the nature of the mass spectrum.

In the multiple goldstini scenario, the spectrum consists of a light gravitino as lightest supersymmetric particle (LSP), behaving as a goldstino, and a number of neutral fermions (the pseudo-goldstini) with a mass between that of the LSP and that of the lightest particle of the observable sector (LOSP). I will mostly discuss the case in which we have only one pseudo-goldstino and where the neutralino is the LOSP. The coupling of the LOSP to the pseudo-goldstino can be enhanced with respect to those of the gravitino giving rise to characteristic signatures.

The decay modes of the neutralino LOSP into a photon or a Z-boson and a pseudo-goldstino can be relevant for detection. I will discuss the expected signatures of this model at future e+e- linear colliders and at the LHC.

Gravitino production at LHC

B. Oexl

Vrije Universiteit Brussel – IIHE (ULB-VUB)

We study signals of jets plus missing energy at the LHC in a scenario where the gravitino is the lightest supersymmetric particle and the gluino is the next-to-lightest supersymmetric particle which promptly decays into a gluon and a gravitino. The signals are produced via associated light gravitino productions with a gluino and/or gluino pair productions, depending on the gravitino and the gluino masses. By merging matrix elements with parton shower, we generate inclusive signal samples and show that the kinematical distributions of the jets and missing transverse energy can explore the gluino mass, while the jet multiplicities provide information about the gravitino mass.

D7 [BP7] Contributed Lecture Particle and Nuclear Physics

Phenomenology of Scalar Top Pair-Production at the LHC

Thomas in't Veld*

Master student KULeuven PHENO group VUB

Phenomenology of beyond-the-Standard-Model physics is a rapidly evolving domain due to the enormous amounts of data being collected by, among others, the Large Hadron Collider. In the past decade, various tools have been developed to simulate and test the various theoretical models in an experimental context; with tools like MadGraph/MadEvent1 and FeynRules2. we now have a very efficiënt way to complete the chain from theoretical to experimental particle physics.

Supersymmetry is still one of the more satisfying symmetries to extend the Standard Model with. Although the parameterspace for viable supersymmetric extensions of the Standard Model has been ever shrinking with increasing data from collider experiments, there are still very good reasons to investigate SUSY models (like for instance the hierarchy problem for the Higgs boson mass, dark matter candidates, and the uni cation of coupling constants at high energies).

Various models of supersymmetry breaking induce different mass spectra of superparticles; where in most sce- narios the neutralino is the lightest supersymmetric particle (or LSP) and the superpartner of the top quark (the scalar top or stop) is the next-to-lightest susy particle (or NLSP). We investigate scenarios for different masses of the stop and the neutralino, and study hadron collision processes where a pair of scalar tops is produced - with the stops subsequently decaying to neutralinos and Standard Model top quarks.

We will discuss relevant experimental observables to differentiate a supersymmetric scalar top pair-production from the standard model background (pair-production of top quarks).

D8 [BP5] Poster Particle and Nuclear Physics

Muon Counting study using IceTop

Haj Ismail

Universiteit of Ghent

Construction of IceCube, a cubic kilometer neutrino detector, was completed at the end of 2010. It consists of 5160 digital optical modules (DOMs) distributed over 86 strings buried between 1450 and 2450m deep in the Antarctic ice at the South Pole. The surface component of IceCube is the extensive air shower array, IceTop. IceTop consists of 81 stations over 1km^2 area. Each station has two cylindrical tanks placed 10m from each other and filled with ice. Each tank contains two DOMs to detect the Cherenkov radiation emitted by charged particles created in the ice.

IceTop is used to study charged cosmic rays with energies between 100TeV and 1EeV. Cosmic ray air showers are dominated by electrons and muons at the ground level. In this poster we will show an overview of the method we use to extract the muon contribution from the total signal created by all particles in the shower and use it to study the chemical composition of cosmic rays.

Characterization of BEGe detectors in the HADES underground laboratory in view of their application to neutrinoless double beta decay searches

Erica Andreotti[1] for the GERDA collaboration

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A complete characterization of newly produced Broad Energy Germanium detectors (BEGe), enriched in the isotope ^{76}Ge, is being carried out in the HADES underground laboratory, located 225 m below ground in Mol (Belgium). These detectors have been produced in the context of the GERDA experiment, searching for the neutrinoless double beta decay of ^{76}Ge. An important feature of BEGe detectors is their enhanced pulse shape discrimination, which allows in particular discriminating neutrinoless double beta decay from gamma-ray background events.

The aim of the characterization consists in the determination of all the important operational parameters of such detectors, like the active volume, the dead layer thickness and uniformity over the surface and to test the performance of the diodes in terms of energy resolution and quality of pulse shape discrimination.

The tests are being performed in the HADES underground laboratory in order to minimize the germanium exposure to cosmic radiation and the consequent activation, which could otherwise increase the intrinsic background of the detectors. The sand-clay overburden of about 500 m water equivalent assures in fact a muon flux reduction factor of about 5000 [1]. Two types of mechanical set-ups have been designed for the tests and deployed to the HADES underground laboratory, where a dedicated area has been allocated. One type consists of a simple measurement table, with a lead shield surrounding the detector, suitable for measurements with a test source placed in fixed positions (collimated or uncollimated). A second one is provided with a movable, motor controlled arm, which allows performing an automatized full area scanning of the diode with a collimated source. The latter is particularly suited for determining the dead layer thickness and uniformity of the whole surface, in order to detect any potential charge collection deficiency. Automatized acquisition systems, both analog (MCA) and digital (FADC), will be run in parallel in order to fully exploit the features of both systems.

This work aims at describing the characterization procedure and the measurement setups, as well as the preliminary results obtained and the potential applications which can be derived.

References

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[http://www.kinr.kiev.ua/NPAE-Kyiv2010/html/Proceedings/8/Andreotti.pdf].

DOSE AND RADIATION EFFECTS ASSESSMENT DURING FUTURE MISSIONS TO THE MOON AND MARS

Emanuele Cazzola1,2, Giovanni Lapenta1

1)Centre for Plasma Astrophysics, Departement Wiskunde, Katholieke Universiteit Leuven 2) Dipartimento Energia, Politecnico di Torino, Torino, Italy

During the upcoming decades, all important worldwide space agencies are planning to undertake interplanetary travels outside the terrestrial magnetic field with the goal of achieving many purposes: from scientific exploration to economical gain. This effort requires to face one of the greatest issues in space: radiation. The present work deals with an investigation on the radiation dose astronauts may receive during two of the most important missions, i.e. the Moon and Mars colonization. Concerning the assessment, the missions are divided into many segments in order to take into consideration all the different radiation sources. The main radiation the astronauts are going to face are SPE – Solar Proton Events and GCR – Galactic Cosmic Rays, since radiation belts around Earth may be neglected due to the short exposure time.

We have developed a new program code, which takes as input particle fluxes recorded by some specific satellites, such as ACE and GOES, and allows the user to choose some principal parameters related to shielding and geometric conditions. As output, the code gives the value of the effective dose and the ambient dose equivalent, both expressed in Sievert, as also addressed by recent radiation protection commissions pubblications.

Furthermore, there will be the chance to make the code available online, in order to allow online users to access it.

D11 Poster Particle and Nuclear Physics

Search for Secluded Dark Matter with the IceCube Neutrino Telescope

J. Miller

Vrije Universiteit Brussel – IIHE (ULB-VUB)

Interest has developed in models where dark matter is secluded from the Standard Model via a mediator. Dark matter may be gravitationally captured in the Sun and annihilate into a non-Standard Model mediator, which subsequently decays into Standard Model particles and may decay in the vicinity of the Earth. In some models the result from such a decay, close co-linear muons, can be a unique signal in a neutrino telescope, such as the IceCube detector at the South Pole. A potential signal can be discriminated from atmospheric neutrinos via the energy deposition topology in the detector. We present the status of secluded dark matter searches with the 79-string IceCube configuration.

PARALLEL SESSION (E)

MEDICAL PHYSICS AND BIOPHYSICS

Auditorium D.0.05, 15:00 – 17:45

Chairman: Patrick Wagner (Universiteit Hasselt)

<u>Invited lectures:</u>

	15:00 – 15:35	"Electrical monitoring of charged macromolecules by means of field-effect devices: Possibilities and limitations"	M. Weil Univ. of Applied Sciences, Kaiserslautern
	15:35 – 16:10	"Accurate and fast simulation of channel noise in models of biological neurons"	M. Giugliano Univ. Antwerpen
	16:10 – 16:45	"Physics in DNA hybridization and its relevance for diagnostic applications"	J. Hooyberghs VITO, Mol

<u>Contributed Lectures:</u>

E1	16:45 – 17:00	"Probing hybridization parameters from microarray experiments: nearest neighbor model and beyond"	W.-W. Hadiwikarta VITO, Mol
E2	17:00 – 17:15	"Heat-transfer resistance at solid-liquid interfaces: A tool for the detection of single nucleotide polymorphisms in DNA "	B. van Grinsven Univ. Hasselt
E3	17:15 – 17:30	"MIP-based biomimetic sensor for the electronic detection of serotonin in human blood plasma"	M. Peeters Univ. Hasselt
E4	17:30 – 17:45	"NMR Theory of longitudinal and transverse relaxation times induced by superparamagnetic particles "	Q. L. Vuong Univ. Mons

Physics in DNA hybridization and its relevance for diagnostic applications

J. Hooyberghs

VITO, Mol

DNA hybridization is the binding of complementary single stranded sequences to form a double helix. It is a fundamental process in many DNA measurement techniques. The thermodynamical aspects of DNA hybridization is fairly well understood for the specific case when both strands are in solution (i.e. in a bulk liquid far from any surface). Models are known for accurate prediction of the sequence- and temperature-dependent free energy. However, in many technological applications hybridization occurs between sequences in solution and surface-bound sequences. Even though the technology may be mature, like that of microarrays, the knowledge of the underlying physical properties is not.

The presentation will explain the principles of a microarray and the physics behind DNA hybridization. It will show how the use of microarrays allows the free energy quantification of DNA hybridization and how it provides insight into the kinetics of the hybridization process which turns out to be important for the specificity of the sequence detection. As an explicit example the detection of point mutations in DNA will be discussed together with a relevant case study in medical diagnostics.

Electrical monitoring of charged macromolecules by means of field-effect devices: Possibilities and limitations

M. Weyl

University of Applied Sciences Kaiserslautern

Label-free detection of molecular interactions utilizing field-effect devices is one of the most attractive approaches for a new generation of biochips with direct electrical readout for a fast, simple and cost-effective analysis. Capacitive electrolyte-insulator-semiconductor (EIS) sensors are promising tools for the label-free electrical detection of charged macromolecules via their intrinsic charge. Polyelectrolyte multilayers (PEM) and DNA molecules have been utilized as model systems to study the charge effects induced in EIS sensors by the formation of "planar"- and "brush"-like molecular layers, respectively.

The sequential adsorption of oppositely charged PE layers induces interfacial potential changes, resulting in alternating shifts of the capacitance-voltage (C-V) curves and constant-capacitance (ConCap) signal of the EIS sensor. The direction of the signal changes depends on the charge sign of the outermost PE layer. Moreover, the potential shifts have a tendency to decrease with increasing the number of adsorbed PE layers and ionic strength of the solution, whereas the decay is stronger and started earlier at higher salt concentrations.

In addition, an array of on-chip integrated nanoplate EIS sensors has been developed, enabling the reliable detection of DNA hybridization/denaturation in a differential measurement setup. Enhanced DNA biosensor characteristics were achieved by using low-concentrated buffer solution for the measurements. Furthermore, an electrostatic model for an EIS sensor modified with "planar"- and "brush"-like molecular layers was developed. The model predicts a strong dependence of the sensor signal on the electrolyte concentration, surface charge density and the distance between the charged layer and the sensor surface. This is consistently agreeing with the experimental results.

Invited Lecture Medical Physics and Biophysics

Accurate and fast simulation of channel noise in models of biological neurons

Michele Giugliano

Antwerp University, Department of Biomedical Sciences, Belgium

It is today becoming increasingly common to complement the experimental study of the brain (dys)functions, by routine mathematical modeling and super-computer simulations. Biophysical accurate descriptions of single neuron excitable properties, as well as of the generation and transmission of nerve impulses across connected neurons, have been constantly refined over the last 60 years. There is currently so much hope on in silico recreations of the brain, that several large scale initiatives are steadily gaining momentum (e.g. see the FP7 Future Emerging Technologies Pilot FlagShip on the "Human Brain Project", the IBM-sponsored Blue Brain Project, the DARPA and IBM-sponsored Cognitive Computing initiative).

An inherent limit of all these approaches is that the biophysical descriptions, considered so far, focus exclusively on average effects of the microscopic components of cell membrane ion permeability and excitability: voltage- and ligand-gated ion channels. Since the 70s, we know however that random gating of membrane proteins is a major source of intrinsic neuronal variability and its impact on brain (dys)functions is currently unknown. This non-deterministic components of neuronal electrophysiology can be captured by Montecarlo simulations of Markov models, accounting for individual ion channels. Unfortunately, such a level of details is still out of reach in large scale brain models, due to intrinsic heavy computational requirements inaccessible even from top modern parallel computers.

In this talk, I will review existing Langevin-like generalizations of the classic Hodgkin-Huxley equations that describe neuronal excitability, and provide a novel formulation that reproduces accurately the statistical properties of the exact microscopic simulations. This formulation is extremely interesting as it allows existing large scale simulations to be quickly and efficiently extended to include the stochastic effects of membrane ion permeability. In conclusion, by the analysis of the properties emerging in exact Markov schemes by standard probability calculus, I will show the sources of inaccuracy of previous proposals.

E1 Contributed Lecture Medical Physics and Biophysics

Probing Hybridization parameters from microarray experiments: nearest neighbor model and beyond*

Hadiwikarta, W.W.1,2, Walter, J.-C.2, Hooyberghs, J.1,3, Carlon, E.2

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Nucleic acids (de-)naturation is essential in many biophysical systems [1]. It occurs in living cells and is being used in different hybridization-based biotechnological applications, i.e. PCR, microarrays, etc.. It is important to understand its thermodynamics properties both because of technological relevance and of scientific interest. Here we present a method based on optimized and dedicated DNA microarray experiments to assess these properties. We found that the data is in line with the theoretically expected equilibrium isotherms [2]. By a thorough analysis, we succeeded in quantifying the free-energy penalties of mismatches (non-Watson-Crick pairs). Moreover we evaluated the range over which two mismatches in a helix could interact and studied the effect of mismatches close to the edge of the helix. Their extra penalties were also quantified. Further analysis on our data revealed some energetic outliers that could be influential in studying structural conformation change due to mismatches.

These results provide new insights on the DNA hybridization and can help to increase the accuracy of hybridization-based technologies.

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[2] Hooyberghs, J., Van Hummelen,P., and Carlon, E., The effects of mismatches on hybridization in DNA microarrays: determination of nearest neighbor parameters, Nucleic Acids Res., 37, e53, (2009).

Heat-Transfer Resistance at Solid-Liquid Interfaces: A Tool for The Detection of Single Nucleotide Polymorphisms in DNA

Bart van Grinsven [1], Natalie Vanden Bon [2], Hannelore Strauven [1], Lars Grieten [1],
Mohammed Murib [1], Kathia L. Jiménez M. [1], Stoffel D. Janssens [1,3], Ken Haenen [1,3],
Michael J. Schöning [4],
Veronique Vermeeren [2], Marcel Ameloot [2], Luc Michiels [2], Ronald Thoelen [1,5],
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Abstract: In this work, we would like to report on the heat-transfer resistance at interfaces as a novel, denaturation-based method to detect single-nucleotide polymorphisms in DNA. We found that a molecular brush of double stranded (ds) DNA grafted onto synthetic-diamond surfaces does not notably affect the heat-transfer resistance at the solid-to-liquid interface. However, molecular brushes of single stranded DNA cause a substantially higher heat-transfer resistance and behave like a thermally insulating layer. This effect can be utilized to identify ds-DNA melting temperatures *via* the switching from low- to high heat-transfer resistance. The melting temperatures identified with this method for different DNA duplexes (29 base pairs without and with built-in mutations) correlate nicely with data calculated by modelling. The method is fast, label-free (without the need for fluorescent or radioactive markers), allows for repetitive measurements, and can also be extended towards array formats. Reference measurements by confocal fluorescence microscopy and impedance spectroscopy confirm that the switching of heat-transfer resistance upon denaturation is indeed related to the thermal on-chip denaturation of DNA.

MIP-based biomimetic sensor for the electronic detection of serotonin in human blood plasma

Marloes Peeters [1], F.J. Troost, B. van Grinsven, F. Horemans, J. Alenus, M.S. Murib,

D. Keszthelyi, A. Ethirajan, R. Thoelen, T.J. Cleij, and P. Wagner

1) Hasselt University, Institute for Materials Research IMO,

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Serotonin is an important signaling molecule in the human body. It is involved in a wide variety of biological processes, such as central processes, mood, appetite and gastrointestinal motility [1]. The detection of serotonin is commonly performed by high performance liquid chromatography (HPLC), which is costly and time consuming due to extensive sample preparation. We will show that these problems can be overcome by using molecularly imprinted polymers (MIPs) as synthetic receptors in combination with impedance spectroscopy as readout technique [2]. The MIPs were prepared with several blends of the underlying monomers and the best performing MIP material was selected by optical batch-rebinding experiments. MIP microparticles were then immobilized on polymer-coated electrodes and integrated in an impedimetric sensor cell [3], allowing for simultaneous measurements with a reference channel. Dose-response curves were measured in PBS buffer and in non-diluted blood plasma. The plasma level of healthy persons is 5 – 20 nM and the sensor provides reliable data in this concentration regime as an independent validation by HPLC measurements demonstrates. Finally, we show that the impedimetric response upon serotonin binding can be attributed to a capacitive effect at the interface between the MIP particles and the plasma.

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[3] M. Peeters, F.J. Troost et al., accepted by *Sens. Actuators, B.*

NMR Theory of longitudinal and transverse relaxation times induced by superparamagnetic particles

Q. L. Vuong[1], Y. Gossuin[1], P. Gillis[1], A. Roch[2] and S. Delangre[1]

[1]*Biological Physics Department, UMONS*
[2]*General, Organic and Biomedical Chemistry, UMONS*

Magnetic Resonance Imaging (MRI) has become a widely used medical imaging technique. It is based on Nuclear Magnetic Resonance: nuclear spins – usually, hydrogen proton spins – under a static magnetic field are excited by a radiofrequency field and then return to equilibrium when the excitation source is turned off. This relaxation phenomenon can be characterized by nuclear magnetic longitudinal and transverse relaxation times (T_1 and T_2) which are well known to influence the image contrast in MRI. Magnetic particles, called *contrast agents*, can induce a variation of the voxel intensity in the MR image by shortening the proton relaxation times.

Superparamagnetic particles are single monodomains of ferromagnetic or ferrimagnetic materials. The electron spins of these particles are aligned with each other: an SPM particle has thus a large magnetic moment. SPM particles can be used as T_2-contrast agent: they produce high magnetic inhomogeneities – through their dipolar magnetic field – which quickly dephase the nuclear magnetic moments [1,2]. A study of the physical particle characteristics on the relaxation times leads to the optimal parameters to reach a good contrast agent efficiency and can be used as a characterization method for the magnetic particles.

In this work, a new classical formalism is introduced which allows the simulation of the nuclear magnetic relaxation induced by an aqueous sample of SPM nanoparticles. This formalism is based on a more intuitive understanding of the relaxation by the use of classical vectors. An Inversion Recovery Sequence which produces longitudinal relaxation times T_1 and T_2 sequences (with or without spin echoes) can be simulated at any desired static field. Nuclear Magnetic Resonance Dispersions (NMRD, i.e curves showing the dependence of the relaxation times on the static field) are obtained for particles in and out of the Redfield conditions, i.e. for large SPM magnetization and radii. To our knowledge, this is the first time that such curves are obtained.

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E5 Poster Medical Physics and Biophysics

Lab on a chip: effective immobilization of PT- modified oligonucleotides on the gold surface of DNA chips based on Surface Plasmon Resonance

Jiménez Monroy Kathia L1., Kick Alfred2, Wagner Patrick1, Mertig Michael2 1

IMO- IMOMEC (Universiteit Hasselt), 2 Max Bergmann Center (TU Dresden)

DNA chips or biochips, have allowed the merging of computer chips with biological information obtained from the Human Genome Project (HGP). A DNA chip is a device where many DNA sensors are integrated on the same surface; this is analogous to the concept of high density of electronic circuits on a microchip.

DNA chips are currently applied for gene discovery and expression, mapping genomic libraries, as well as a tool for detecting mutations and polymorphisms. Moreover, these devices need to be streamlined and optimized before they are ready for routine clinical use. To develop a DNA array, it is necessary to take into account three main factors: the probe to be used as the biorecognition element, the arraying technique and the detection method for the hybridization event.

The standard procedure consists of a thiol- (SH) modified probe to immobilize oligonucleotides onto a gold surface, in which a strong bond between sulfur and gold is formed. Taking into account that phosphorothioate- (PT) modified oligonucleotides have been proved to have a higher stability in presence of endonucleases, PT- probes were used as well for immobilization.

This project is focused on the arraying technique, using a covalent attachment of oligonucleotides to a gold surface and analyzed with a novel tool, developed by the Fraunhofer (IOF, Jena, Germany and IWS, Dresden Germany) and Max Bergmann Center (TU, Dresden). It consists of a surface plasmon resonance (SPR) spectrometer which exploits gold coated chips (TOPAS® chip) with integrated optics and microfluidics.

Two different functionalization strategies were done to produce a reactive iodo- alkyl self assembled monolayer (SAM) for the attachment. A nanoliter dispenser was then used to deposit linear and hairpin oligonucleotides in microarrays. These probes contain a single-stranded antitag sequence, which is complementary to a tag sequence, included on the PCR products used for hybridization experiments. Finally, antitag-tag hybridization was analyzed by SPR spectroscopy.

This project reports a successful application of SAMs with iodo-alkyl derivatives to immobilize PT- modified oligonucleotides, compared to PT- modified probes immobilized on bare gold surface. Moreover, the SPR device showed a high sensitivity for immobilized probes on iodine-trimethoxy silane surfaces, being able to detect PCR product concentrations as low as 3.6nM. This optimization in SPR detection could be used in commercial biochips to get readouts in matter of minutes for different immobilized DNA with mutations at different locations in the same chip.

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The use of spatially-controlled metallic nanostructures for biomolecule immobilization

Tobias Peissker1,2, Barbara Gysbrechts1, Gloria Fabris1, Olivier Deschaume1, Danielle R. Rand2, Kelly Houben1, Christian P. Romero1, Carmen Bartic1,2, Margriet J. Van Bael1

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Conserving the biological activity of immobilized biomolecules is an important first step when developing analytical devices such as biosensors. The immobilization approach must be tuned so as to avoid denaturation or steric hindrance between molecules. Here we demonstrate controlled biomolecule immobilization at the nanometer scale by depositing binding sites with high specificity and controlled surface density. Surfaces comprising both protein-repellent and protein-binding areas were prepared in order to obtain a directed immobilization of biomolecules, while simultaneously maintaining their biological activity. To create protein-repellent areas, a polyethylene glycol (PEG)-silane was grafted on a flat SiO2 surface. Surface topography and properties such as protein repellence were characterized by complementary analysis methods, namely atomic force microscopy and spectroscopy (AFM), quartz crystal microbalance (QCM), x-ray photoelectron spectroscopy (XPS) and static contact angle (CA) measurements. Surface analysis by x-ray photoelectron spectroscopy spectra showed the characteristic C - O and C - C/C - H peaks at 283.5 eV and 285 eV, respectively, attributed to PEG moieties [1]. Furthermore, a decrease in surface contact angle and an increase in adhesion force measured by atomic force spectroscopy were observed, indicating the presence of highly hydrated PEG chains on the surface. QCM experiments revealed that non-specific protein adsorption to the SiO2/PEG-silane surface decreased by approximately 95% compared to a bare SiO2 surface. Next, gold nanostructures in the size range comparable to that of a biomolecule (1-3 nm) were deposited by molecular beam epitaxy and laser-assisted cluster deposition to serve as binding sites for biomolecules [2, 3]. Topographical analysis by atomic force microscopy showed the successful deposition of nanostructures on the PEG-silane surface. In the final step, the nanostructures were functionalized with a linker molecule for the attachment of streptavidin. Thus, our approach demonstrates a method for the controlled deposition of metallic nanostructures on a protein repellent substrate that results in a surface with biologically-relevant nanostructures available for further functionalization.

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E7 Poster Medical Physics and Biophysics

Probing model lipid membranes in interaction with gold nanoparticles by using vibrational sum-frequency generation spectroscopy

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The study of nanotoxicity is a critical issue today since nanoparticles are increasingly used in multiple technological and bio-technological fields. The aim of our study is to characterize, at the molecular scale, the structural changes caused by the gold nanoparticles on the membrane, as well as the interactions occurring at this bio-interface, through the analysis of its vibrational non-linear optical response. The challenge is to take advantage of the intrinsic interface sensitivity of second-order nonlinear optical phenomena to go further into the understanding of the interactions that occur at the interface between nanoparticles and cellular membranes. In fact, the even order non-linear optical phenomena, such as the Sum-Frequency Generation (SFG), are forbidden in centrosymmetric media (such as bulk media), and therefore become intrinsically specific to surfaces and interface, where the inversion symmetry is broken [1].

In this study, we investigate, taking advantage of the high surface sensitivity of the SFG spectroscopy, the interface between model membranes made of a lipid bilayer and spherical gold nanoparticles in a physiological medium. The conception of these model membranes, supported on a solid substrate, can be realized with the well-known Langmuir-Blodgett (LB) and Langmuir-Schaefer (LS) methods [2], or the spontaneous fusion of vesicles (SFV). The non-linear optical response of the interface is measured between 3600 cm-1 and 2800 cm-1, where the stretchings of the interfacial water molecules and of the aliphatic tails of the lipid molecules hold strong physico-chemical information. In particular, we focused here on the analysis of the organization and the stability of these membrane models. It results that these preparation methods all provide highly ordered films regarding the conformation of the lipid aliphatic chains. However, it turned out that SFV bilayers fold on themselves when exposed to air, and irreversibly form domains of mono- and tri-layers of lipids.
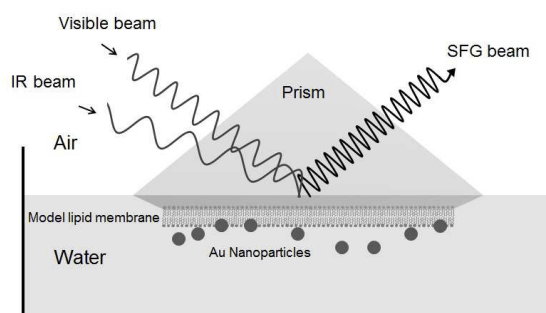

Fig. 1: Schematic representation of a typical SFG measurement on the Au-NPs – membrane model interface. The incident beams are in the total internal reflexion geometry.

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Real-time study of chemically induced DNA denaturation by impedance spectroscopy with NCD-based sensor electrodes

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Diamond has proven to be an excellent platform for biomedical research, due to its excellent material properties such as chemical inertness, thermal conductivity, and electronic properties [1, 2]. In previous work it was established that the monitoring of chemically-induced denaturation at room temperature is an interesting approach to measure DNA duplex stability as an alternative to thermal denaturation at elevated temperatures [3]. Elaborating on these results we now report on the electronic monitoring of DNA denaturation by NaOH, induced at different flowrates (0.05 ml/min to 0.5 ml/min) with variable molarities (0.05 M to 0.5 M), using electrochemical impedance spectroscopy as read out technology. Probe DNA, consisting of a 36-mer fragment was covalently immobilized on nanocrystalline-diamond electrodes and hybridized with different types of 29-mer target DNA (complementary, single-nucleotide defects at two different positions, and a non-complementary random sequence). The mathematical separation of the impedimetric signals into the time constant for NaOH exposure and the intrinsic denaturation-time constants gives clear evidence that the denaturation times reflect the intrinsic stability of the DNA duplexes. The intrinsic time constants correlate with calculated DNA-melting temperatures. The impedimetric method requires minimal instrumentation, is label-free and fast with a typical time scale of minutes and is highly reproducible.

Keywords: Electrochemical impedance spectroscopy, diamond, deoxyribonucleic acid, denaturation time constant, mutation analysis.

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**Structural Imprinting of NR8383 cells, RAW Cells and Saccharomyces
Cerevisae: Potential for Atherosclerosis Screening**

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Centre, 4) IMOMEC division, IMEC vzw

Cardiovascular diseases are still the number one cause of death in Western society. In many cases atherosclerosis plays an important role in causing the disease. The CARIM research center at the University of Maastricht therefore performs a lot of research in the field of atherosclerosis. This research showed that monocytes play an important role in the progression of the disease. Therefore a sensor platform that is able to detect certain phenotypes of monocytes in a specific manner would be a valuable tool in handling atherosclerotic diseases.

The sensor design is based on mass sensitive detection of monocytes; a quartz crystal microbalance (QCM) substrate is coated with a polyurethane polymer layer. The specific recognition of monocytes is based on surface imprinting. After applying the polyurethane layer on the substrate monocytes are pressed into this layer by stamping. Subsequently the layer is cured overnight. In this way the polymerization is completed whit the target cells imbedded into the layer. During crosslinking the curing polymer interacts with functional groups on the surface of the monocytes forming hydrogen bonds between the polymer and the template. Finally the template monocytes are removed from the polyurethane layer by rinsing the substrate with hot water, leaving behind binding cavities showing specificity for the template cells. This specificity is morphological as the size and shape of the cavities are complementary with the template cells form and shape, as well as functional as the template interacts with the polymer during curing. The rebinding of the template to the polyurethane layer is analyzed using a QCM dissipation technique.

In the first phase of the research Saccharomyces cerevisiae are used as template molecules for structural imprinting. These types of yeast cells are less fragile and more abundantly available in comparison to monocytes. The yeast cells were used as model templates to optimize the polyurethane synthesis as well as the imprinting protocol. The substrates were analyzed using optical microscopy and scanning electron microscopy. In the recent past we started optimizing the protocol with living cells as template molecules. RAW cells and NR8383 cells were selected as template molecules because of their similarity to monocytes and the ability to culture these cells in a straightforward manner.

The sensor is designed to be a prototype for future commercially interesting mass produced biosensors. The advantage of using these types of biosensors is that they are far easier and cheaper to produce in comparison to traditional blood test. In comparison to analyzing blood samples in the laboratory, the sensor will give a quick and sensitive measure of the concentration of template monocytes in patient samples. In this way you can quickly determine if a patient is at risk. This will greatly improve the prognosis for the patient and will decrease the risk of sudden deaths caused by these diseases.

PARALLEL SESSION (F)

PHYSICS AND EDUCATION

Auditorium E.0.07, 15:00 – 17:30

Chairman: Marc Debusschere (Science on Stage Belgium)

Workshop

The quest for a conceptual language to support the science integrated curriculum in Flanders; balancing scientific correctness and accessibility.

C. Balck (Kaho St. Niklaas)

The past 5 years science curricula at the secondary school level in Flanders (Belgium) shifted from a one path, subject centered training towards a two- path training including a subject centered path (intended for the future scientist) and a science integrated training (intended for the non scientist, citizen)

This shift in curricula is accompanied by a fundamental shift in methodology.
The science centered approach reduces the observed reality to models and describes and aims to understand this reality using symbols, formulas and mathematics.
Within the science integrated training, reality is observed and described using the mother language, understood and explained conceptually.

Research was conducted to answer the question weather science teachers, until now educated in the science centered system, are able to make this shift in methodology, specifically when teaching about the variables 'force' and 'energy'.
Results exposed specific difficulties encountered in formulating conceptual definitions. Currently conceptual definitions are being developed and tested.

HOW WELL DO THEY LEARN NEWTONIAN MECHANICS CONCEPTS?

PRE- AND POSTTESTING STUDENTS IN A FIRST SEMESTER MECHANICS
COURSE IN THE FIRST YEAR BACHELOR OF SCIENCE.

E. Carette, N. Mennekens and J. Danckaert
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This article presents data on the Force Concept Inventory 2 used as diagnostic test since 2004 in the first year bachelor of Science at the Vrije Universiteit Brussel.

Since the academic year 2004-2005, we have administered the Force Concept Inventory at the beginning of the mechanics course, and after the first exami- nation period in winter. The pretest reflects students initial knowledge about force and motion at the moment of entry at university, the posttest is assumed to reflect their understanding after a one semester university course on New- tonian Mechanics. Data spanning nearly a decade are presented.

REFERENCES
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PARALLEL SESSION (G)

STATISTICAL & MATHEMATICAL PHYSICS

Auditorium E.0.05, 15:00 – 17:30

Chairman: J. Indekeu (Katholieke Universiteit Leuven)

Contributed Lectures:

G1	15:00 – 15:20	"Fluctuation-response relations for nonequilibrium diffusions with memory "	C. Maes K.U. Leuven
G2	15:20 – 15:40	"Modeling of genetic networks via evolutionary algorithms "	M. Van Dorp K.U. Leuven
G3	15:40 – 16:00	"Non-equilibrium response in the boundary driven Lorentz gas "	A. Salazar K.U. Leuven
G4	16:00 – 16:20	"Connecting the von Neumann and Rényi entropy for Fermions "	M. Fannes K.U. Leuven
G5	16:20 – 16:40	"Ising model for distribution networks"	H. Hooyberghs K.U. Leuven
G6	16:40 – 17:00	"Non-local electrodynamics effect on surface superconductivity"	J. Indekeu K.U. Leuven
G7	17:00 – 17:20	"Phase-space dynamics of the quantum Hall state"	D. Sels Univ. Hasselt

G1 Contributed Lecture Statistical & Mathematical Physics

Fluctuation-response relations for nonequilibrium diffusions with memory

C. Maes, S. Safaverdi, P. Visco, and F. van Wijland

(ITF, KU Leuven)

We discuss the extension of the fluctuation-dissipation theorem to nonequilibrium Langevin systems with memory. Simulations in the underdamped case explore the corrections to the Sutherland-Einstein relation in the case of nonequilibrium diffusion, possibly anomalous, in particular for the role of the nonequilibrium forcing and the influence of memory. This relation allows one to access new experimental information regarding active forces in living cells that cannot otherwise be accessed.

(arxiv:1203.3571v1 [cond-mat.soft]).

G2 Contributed Lecture Statistical & Mathematical Physics

Modeling of genetic networks via evolutionary algorithms

Matthijs Van Dorp

(ITF, KU Leuven)

In living cells genes, mRNA and proteins interact via direct and feedback mechanisms so as to form complex networks, known as Gene regulatory networks (GRNs). The organization of genes and proteins into GRNs allows a cell to perform complex tasks and to respond adequately to changes in the environmental conditions. Nowadays, as more experimental results become available, there is a lot of interest in the modeling and analysis of these networks.

We present an approach using evolutionary algorithms, which allows to automatically generate networks that provide a desired type of behavior. We discuss the properties of such an algorithm, and the associated possibilities and limitations. We illustrate the potential of the algorithm with a few examples of generated networks that exhibit nonlinear oscillations.

G3 Contributed Lecture Statistical & Mathematical Physics

Non-equilibrium response in the boundary driven Lorentz gas

Alberto Salazar

(ITF, KU Leuven)

We present a numerical study of the response function performed in a boundary driven Lorentz Gas slab (BDLGS) in non-equilibrium stationary states (NSS). Specifically, we study the particle number change due to a moderate shift of chemical potentials in both reservoirs during the NSS, which are achieved by placing the system among thermochemical reservoirs with different densities and uniform temperature. The response function studied here provides an instance of a fluctuation dissipation relation but applied to an NSS. Such extension involves the evaluation of the so-called dynamical activity in the correlation functions. Generally speaking in non-equilibrium processes, a study of such a quantity is in fact a complementary task to the evaluation of entropy fluxes.

Connecting the von Neumann and Rényi entropy for Fermions

Nicholas Van Ryn and <u>Mark Fannes</u>

(ITF, KU Leuven)

There are, up to now, only a few classes of shift-invariant states of infinite quantum spin systems that can be explicitly parametrized and that admit an easy computation of local observables. Finding their mean von Neumann entropy is an important open problem and a necessary step to use them in variational principles. Their integer-order mean Rényi entropies are, however, much more accessible and one may wonder whether they determine the von Neumann entropy and, if so, how to establish the connection. We show that this is possible for Gaussian Fermionic states and provide some explicit controlled approximation schemes.

Ising model for distribution networks

H. Hooyberghs[1], S. Van Lombeek[1], C. Giuraniuc[1,2], B. Van Schaeybroeck[1,3]
and J.O. Indekeu[1]

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2) Institute of Medical Sciences,University of Aberdeen, Aberdeen, UK
3) Koninklijk Meteorologisch Instituut (KMI), Brussels, Belgium

An elementary Ising spin model is proposed for demonstrating cascading failures (breakdowns, blackouts, collapses, avalanches, ...) that can occur in realistic networks for distribution and delivery by suppliers to consumers. A ferromagnetic Hamiltonian with quenched random fields results from policies that maximize the gap between demand and delivery. Such policies can arise in a competitive market where firms artificially create new demand, or in a solidary environment where too high a demand cannot reasonably be met. Network failure in the context of a policy of solidarity is possible when an initially active state becomes metastable and decays to a stable inactive state. We explore the characteristics of the demand and delivery, as well as the topological properties, which make the distribution network susceptible of failure. An effective temperature is defined, which governs the strength of the activity fluctuations which can induce a collapse. Numerical results, obtained by Monte Carlo simulations of the model on (mainly) scale-free networks, are supplemented with analytic mean-field approximations to the geometrical random field fluctuations and the thermal spin fluctuations. The role of hubs versus poorly connected nodes in initiating the breakdown of network activity is illustrated and related to model parameters.

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Non-local electrodynamics effect on surface superconductivity

T. Van Cauteren and J.O. Indekeu

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Effects of non-local electrodynamics on surface superconductivity in type-I superconductors in zero magnetic field are predicted, employing the Ginzburg-Landau (GL) theory as the local approximation. A perturbation expansion in the ratio of the Pippard (or BCS) coherence length and the temperature-dependent GL coherence length of superconductivity is set up. For materials with surface enhancement of superconductivity, characterized by a negative GL surface extrapolation length b and by a surface critical temperature Tcs that exceeds the bulk Tc, an additional increase of Tcs is predicted. Calculations to first order in the perturbation parameter show that about 13% of the recently measured difference Tcs −Tc ≈ 0.05K in a surface-enhanced Sn film, is attributable to a non-local electrodynamics effect [1].

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Phase-space dynamics of the quantum Hall state

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Theory of quantum and complex systems, Physics Department,
Universiteit Antwerpen

In the realm of Ehrenfestís theorem, classical trajectories obeying Newtonís laws have been proven useful to construct explicit solutions to the time-dependent WignerñLiouville equation[1][2]. Recently we extended this method by constructing the real time propagator for the Wigner distribution funtion as a phase space path integral[3]. By analogy with the Feynman path integral we deÖne a new e§ective action of the system in the Wigner-Weyl representation. After properly incorporating the e§ects of an applied magnetic Öeld and possible geometric constraints on the particles motion, we were able to Önd a solution for the integer quantum Hall e§ect in terms of classical phase-space trajectories.

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