BOOK OF ABSTRACTS

XXXVI
INTERNATIONAL SYMPOSIUM
DYNAMICAL PROPERTIES OF SOLIDS
Cracow, 27 – 31 August 2017

Tomasz M. Majka
Publisher

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DyProSo is an international biannual research meeting on functional properties of condensed matter resulting from elementary excitations, molecular motions, transport processes and other dynamic phenomena occurring in many body systems. Of special concern is always a scientific dialogue between young and experienced researchers working on the dynamics of materials. The 36th DyProSo will be held in Cracow, a historical site known as not having been "built in a day", in the year of Marian Smoluchowski

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Foreword

Dear Participant,

We are pleased to welcome you to the 36th International Symposium on Dynamical Properties of Solids. This time the event is held in Cracow and is organized jointly by three institutions: The Henryk Niewodniczański Institute of Nuclear Physics of Polish Academy of Sciences (IFJ PAN), The Cracow University of Technology (CUT) and The Pedagogical University of Cracow (PUC). The year 2017 marks the 100th anniversary since the death of Marian Smoluchowski. Therefore we would like to meet you at a reception in the Collegium Witkowski of the Jagiellonian University, the M. Smoluchowski's last place of work. For the other sessions we invite you to the former palace Łobzów housing nowadays the Faculty of Physics, Mathematics and Computer Science of CUT. To enable as many as possible young researchers to gain experience in speaking in front of an international public we have arranged sessions of short scientific communications. The periodical Nature Physics will award a prize for the best student communication and for the best poster. Because the matter of the dynamics of solids is growing beyond a pure science a session "Applications and interdisciplinary subjects" will complete the traditional themes of the DyProSo meetings. We thank Professor Marek Stankiewicz for agreeing to present the Polish National Centre of Synchrotron Radiation and the growing experimental potential of the facility. Cracow is known as not having been "built in a day". It is, thus, readily impossible to visit all its interesting historical vestiges even within a week. Nevertheless, we will show you the oldest existing College of the 653-year-old Jagiellonian University and invite you, after a short site-seeing walk, to the conference dinner in the Jewish quarter Kazimierz. We thank all the invited speakers for accepting our invitation and all the participants for their interest in the event. We wish you fruitful and stimulating discussions and a nice stay in Cracow.

Renata Bujakiewicz-Korońska
Renata Bujakiewicz-Korońska
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Previous DyProSo conferences

1	1967	Albe, France
2	1968	Oberwolfach, Germany
3	1969	Mont Saint-Odile Nancy, France
4	1970	Oberwolfach, Germany
5	1971	Edinburgh, UK
6	1972	Montpellier (Mont Aigoual), France
7	1973	Leoni (Starnberger See), Germany
8	1974	Giswil, Switzerland
9	1975	Pelvous, France
10	1976	Reading, UK
	1977	Phonon Conference in Paris, France
11	1978	Stresa, Italy
	1979	Ferroelectricity Conference in Edinburgh, UK
12	1980	Le Houches, France
13	1981	Überlingen, Germany
14	1982	San Miniato, Italy
15	1983	Leuven, Belgium
16	1984	Mürren, Switzerland
	1985	Phonon Conference in Budapest, Hungary
17	1986	Überlingen, Germany
18	1987	Ventron, France
19	1988	Sestri, Cinque Terri, Italy
	1989	Phonon Conference in Heidelberg, German
20	1990	Chexbres, Switzerland
21	1991	Autrans, France
22	1992	Schellerau (Dresden), Germany
23	1993	Lunteren, The Netherlands
24	1994	Il Ciocco, Italy
25	1995	Haro (Bilbao), Spain
	1996	(Crete, Greece - cancelled)
26	1997	Davos, Switzerland
27	1999	Tours, France
28	2001	Kerkrade, The Netherlands
29	2003	Trieste, Italy
30	2005	Ceský Krumlov, Czech Republic
31	2007	Porto, Portugal
32	2009	Antwerp, Belgium
33	2011	Aussois, France
34	2013	Vienna, Austria
35	2015	Freising, Germany

Conference programme

Sunday 27 VIII	**The Collegium Witkowski, Jagiellonian University, 13 Gołębia Street**
13:00 – 17:00	***Registration***
17:00 – 17:20	***Opening Ceremony***
17:20 – 18:05	***Opening Lecture*** **Józef Spałek** *Many particle physics: From Smoluchowski to the quantum strongly correlated matter*
18:05 – 20:30	***Welcome Party***
Monday 28 VIII	**Palace Łobzów, Faculty of Physics, Cracow University of Technology, 1 Podchorążych Street**
8:00 – 9:00	***Registration***
9:00 – 9:25	***Invited Lecture*** **Björn Wehinger** *Modern approaches probing phonons with X-rays: Magneto-elastic waves in quantum magnets and the full elasticity tensor from thermal diffuse scattering*
9:25 – 9:50	***Invited Lecture*** **Andreas Tröester** *DFT meets Landau: A finite strain Landau theory of high pressure phase transitions*
9:50 – 10:05	**Matthew Krzystyniak** *Mass-resolved neutron spectroscopy*
10:05 – 10:20	**Jiří Hlinka** *Alternative approaches to zeros and poles of dielectric function – beyond the harmonic phonons*
10:20 – 10:35	**Ivan Gregora** *Raman and IR-active coupled modes in GaV4S8*
10:35 – 10:45	**Matthias Gutmann** *Phonons from neutron diffraction*
10:45 – 11:15	***Coffee Break***
11:15 – 11:40	***Invited Lecture*** **Catalin Gainaru** *Dielectric relaxation processes in glassy and liquid water*
11:40 – 11:55	**Andrzej Budziak** *Influence of doping on the absorption of hydrogen in AB5 – type intermetallic compounds*
11:55 – 12:10	**Vasily Artemov** *A unified mechanism of dielectric relaxation in water and ice*
12:10 – 12:20	**Robert Gębarowski** *Langevin dynamics and sedimentation of nanoparticles*
12:20 – 12:35	**Zbigniew Łodziana** *Ionic conductivity in Metal-closo-Borates*
12:35 – 12:50	**Aristea Maniadaki** *Dynamical properties of closo-Boranes*
12:50 – 13:05	**Andrzej Molak** *Electric relaxations in nitrogen-doped bismuth manganite ceramics*
13:05 – 14:00	***Lunch Break***

Conference programme

14:00 – 14:10	**Izabela Biało** *Inelastic X-ray scattering study of the electron-phonon anomalies in Nd2-xCexCuO4*
14:10 – 14:20	**Łukasz Dubiel** *Temperature dependence of the EMR spectra for Ni50-xCoxMn35.5In14.5 Heusler alloys obtained by melt-spinning process*
14:20 – 14:30	**Fabio Figueiras** *Synthesis of narrow band gap perovskite Ba(Zn,Ti)O3 ferroelectric thin films for environmental friendly photovoltaic conversion*
14:30 – 14:40	**Peio Garcia Goiricelaya** *Suppressed electron-phonon coupling due to strong spin-orbit interaction at the Tl/Si(111) surface*
14:40 – 14:50	**Katharina Holzweber** *Beam-induced atomic motion in oxide glasses*
14:50 – 15:00	**Grzegorz Jagło** *Lattice dynamics of a quasi-2D layered TlCo2Se2 with a helical magnetic structure*
15:00 – 15:10	**Jochen Kalt** *Confined lattice dynamics in ultrathin Ge/Fe3Si/GaAs heterostructures*
15:10 – 15:20	**Magdalena Krupska** *High stability of magnetite thin films under high-energy ion irradiation*
15:20 – 15:30	**Rafał Kuna** *Composition dependence of selected mechanical properties of (Pb,Cd)Te crystal lattice*
15:30 – 15:50	**Marek Stankiewicz** *Synchrotron Solaris*
15:40 – 16:25	***Coffee Break***
16:25 – 16:50	***Invited Lecture*** **Alexei Sokolov** *Tuning dynamic properties of polymer nanocomposites*
16:50 – 17:05	**Małgorzata Jasiurkowska-Delaporte** *Effects of confinement on molecular dynamics of glass forming-liquids*
17:05 – 17:20	**Natalia Osiecka** *Complementary study of solid state polymorphism in ethosuximide*
17:20 – 17:35	**Ewa Juszyńska-Gałązka** *Thermodynamic and dynamic properties of glass of disordered phases*
17:35 – 17:50	**Andriy Kityk** *Molecular ordering and relaxation dynamics in liquid crystal based nanocomposites*
17:50 – 18:05	**Paweł Karbowniczek** *Structure formation in two-dimensional systems of bent-core particles*
18:05 – 19:20	***Poster Session - odd numbers***
Tuesday 29 VIII	**Palace Łobzów, Faculty of Physics, Cracow University of Technology, 1 Podchorążych Street**
8:00 – 9:00	***Registration***
9:00 – 9:25	***Invited Lecture*** **Annette Bußmann-Holder** *Nonlinear spin-lattice coupling in EuTiO3: novel two-dimensional magneto-optical device for light modulation*

9:25 – 9:40		**Jarosław Jędryka** *Nonlinear optical diagnostic of the condensed matter*
9:40 – 9:50		**Gabriela Lewińska** *Polymers for ternary organic solar cells*
9:50 – 10:00		**Grigory Arzumanyan** *Photo- and upconversion luminescence in glass-ceramics doped with rare earth elements*
10:00 – 10:15		**Joaquim Agostinho Moreira** *Structural and vibrational signature of the suppression of cooperative Jahn-Teller distortion in TbMn1-xFexO3*
10:15 – 10:25		**Paweł Śliż** *Phonon spectra of the HgTe-based topological insulators*
10:25 – 10:35		**Andrzej Wal** *Electrons in a finite two-dimensional system*
10:35 – 10:50		**Urszula Wdowik** *Role of spin-orbit interaction and strong electron correlations in predicting fundamental properties of advanced nuclear fuel materials for generation-IV reactors*
10:50 – 11:15	***Coffee Break***	
11:15 – 11:40	***Invited Lecture***	**Marek Paściak** *Low-frequency dynamics in Pb-based ferroelectric relaxors*
11:40 – 11:55		**Jan Petzelt** *Soft and central mode dynamics in relaxor ferroelectric PbMg1/3Nb2/3O3: dielectric response compared to hyper-Raman and neutron scattering*
11:55 – 12:10		**Stanislav Kamba** *Electromagnons in multiferroics with Y- and Z-type hexaferrite structures*
12:10 – 12:20		**Martin Kempa** *Relaxations in uniaxial relaxor ferroelectric SBN*
12:20 – 12:35		**Grażyna Bator** *Switchable perovskite-like crystals with the organic guest*
12:35 – 12:45		**Renata Bujakiewicz-Korońska** *Dynamic properties of Co doped barium titanate*
12:45 – 14:00	***Lunch Break***	
14:00 – 14:10		**Dominika Kuźma** *Spin waves in low dimensional inhomogeneous nanostructures*
14:10 – 14:20		**Jon Lafuente-Bartolome** *Relativistic response and coupled spin-charge plasmon at the Tl/Si(111) surface*
14:20 – 14:30		**Marcin Majka** *Dynamics of arteries – effects of occlusions and embolus*
14:30 – 14:40		**Karolina Martinson** *Weber-Fechner law in short time acoustic pulses*
14:40 – 14:50		**Maria Podgórna** *Raman scattering investigations of phase transitions in the nanocrystals of PbZrO3-BiFeO3 system*
14:50 – 15:00		**Sabine Puchberger** *Ferroelastic domain boundary movement in PbZrO3*

15:00 – 15:10	**Tomasz Skóra** *Theoretical inquiry into the signatures of coherent wavepacket motion in singlet exciton fission*
15:10 – 15:20	**Anna Szeremeta** *Relaxation processes occurs in (1-x) 70/30 PZT - (x) BiMn2O5 ceramics*
15:20 – 15:30	**Daria Szewczyk** *Peculiar thermal transport of 1-fluoroadamantane*
15:30 – 15:40	**Anton Tuluk** *Impedance spectra of the Na0.5Bi0.5TiO3 single crystals and ceramics*
15:40 – 15:50	**Rui Vilarinho** *Correlation of the magnetic structure modulation with the magnetoelectric behavior of TbMn0.98Fe0.02O3*
15:50 – 16:25	***Coffee Break***
16:25 – 16:50	***Invited Lecture*** **Stéphane Rols** *Hydrogen motions in defective graphene: the role of surface defects*
16:50 – 17:05	**Zoryana Usatenko** *Polymers with different topologies in confined geometries*
17:05 – 17:15	**Natalia Nosidlak** *Ellipsometric study of thin films*
17:15 – 17:30	**Marek Przybylski** *Dynamics of isolated hard nanoparticles stabilized by organic ligands as seen by Mössbauer spectroscopy*
17:30 – 19:00	***Poster Session - even numbers***
19:00 – 19:30	***Meeting of International Advisory Board***
Wednesday 30 VIII	**Palace Łobzów, Faculty of Physics, Cracow University of Technology, 1 Podchorążych Street**
8:00 – 9:00	***Registration***
9:00 – 9:25	***Invited Lecture*** **Svetoslav Stankov** *Lattice dynamics of rare-earth silicide nanostructures*
9:25 – 9:40	**Radosław Strzałka** *The influence of phonons and phasonic flips on the structure factor of quasicrystals*
9:40 – 9:55	**Wojciech Szuszkiewicz** *Low-temperature phonon anharmonicity in PbTe and (Pb,Cd)Te solid solution*
9:55 – 10:10	**Kamil Tokár** *Control of vibrational properties of multilayer phosphorene*
10:10 – 10:25	**Paweł Jochym** *Not so giant anharmonicity in PbTe*
10:25 – 10:50	***Invited Lecture*** **Krzysztof Parliński** *Phonon anharmonicity*
10:50 – 11:15	***Coffee Break***
11:15 – 11:30	**Dominik Legut** *Search for superhard materials - importance of the lattice dynamic calculations*
11:30 – 11:40	**Paweł Sobieszczyk** *Total transmission of elastic waves at solid-solid interface*

11:40 – 12:05	***Invited Lecture*** **Zach Evenson** *Atomic-scale dynamics in liquid semiconductor alloys*
12:05 – 12:20	**Agnieszka Chrzanowska** *Solid or fluid?*
12:20 – 12:35	**Łukasz Laskowski** *Porous silica templated nanomaterials for electronics and IT technologies*
12:35 – 13:35	***Lunch Break***
16:30 – 19:30	***Excursion*** *Starting point: The Collegium Witkowski, 13 Gołębia Street*
19:30 – 22:00	***Conference Dinner*** *Szara Kazimierz Restaurant, 39 Szeroka Street*
Thursday **31 VIII**	**Palace Łobzów, Faculty of Physics, Cracow University of Technology,** **1 Podchorążych Street**
8:00 – 9:00	***Registration***
9:00 – 9:25	***Invited Lecture*** **Andreas Borgschulte** *Applications of the Raman effect: From femtosecond spectroscopy to waste water analysis*
9:25 – 9:50	***Invited Lecture*** **Martin Müller** *Fractional dynamics in silkworm silk and spider silk*
9:50 – 10:00	**Adam Szmagliński** *Properties of localized protons in neutron star matter at finite temperatures for realistic nuclear models*
10:00 – 10:25	***Invited Lecture*** **Vincenzo Guidi** *Gas sensing via chemoresistive effect in nanostructured semiconductors*
10:25 – 10:40	**Giacomo Gadda** *A 1D-0D model for the simulation of the cerebral and extra-cerebral flows and pressures*
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11:10 – 11:35	***Invited Lecture*** **Federico Montoncello** *Softening of spin waves calculated under a Hamiltonian approach: importance for information delivery, and in the understanding of reversal avalanches in macrospin networks*
11:35 – 12:00	***Invited Lecture*** **Maciej Krawczyk** *Nanoscale control of spin wave dynamics in ferromagnetic films*
12:00 – 12:10	**Jarosław Kłos** *Spin wave refraction on the interface of uniform and patterned magnetic layers*
12:10 – 12:25	**Mirosław Łabuz** *Short Heisenberg magnets - an insight into the two spin deviations sector*
12:25 – 12:40	**Zbigniew Tomkowicz** *Dynamic Magnetic Properties of the Ferromagnetic Quasi 1D Ising System [Co(NCS)2L2]n ; L=pyridine*

12:40 – 12:55	**Yevhen Zabila** *Study of Bi properties on polymer substrate: a route toward flexible magnetic sensor*
12:55 – 13:10	**Michał Krupiński** *Magnetic transition from dot to antidot regime in large area arrays with perpendicular magnetization*
13:10 – 13:25	***Conference Closing***
13:25 – 14:25	***Lunch Break***

List of posters

1. **Petr Bednyakov**
   High dielectric response in rhombohedral phase of BaTiO3 single crystals
2. **Renata Bujakiewicz-Korońska**
   Orientation of the electric field gradient and ellipticity of the magnetic cycloid in multiferroic BiFeO3
3. **Dominik Czernia**
   Magnetic relaxations in trinuclear complex [TbIII(ZnIIL)2]CF3SO3 induced by applied static magnetic field
4. **Krzysztof Danel**
   A-D-A-type 9,10-bis(phenylethynyl)anthracenes (BPEAs) for small molecule organic solar cells
5. **Iñigo Etxebarria**
   Computational study of the vacancy order in 2/1 mullite
6. **Piotr Fornal**
   Mössbauer spectroscopy in the studies of sedimentation of Fe2O3 in water solution of sugar
7. **Adrien Girard**
   Diffuse scattering at ID28 ESRF side station : a new tool for lattice dynamics studies
8. **Natalia Górska**
   Phase transitions and molecular dynamics of ionic coordination compounds of the[M(DMSO)6](BF4)3 type, where M = V and Fe
9. **Natalia Górska**
   Thermal properties and molecular dynamics of triblock semifluorinated n-alkanes probed by temperature-dependent infrared absorption spectroscopy
10. **Piotr Graczyk**
    Optimizing acoustic wave – spin wave resonant coupling in the magphonic crystal
11. **Alexandre Ivanov**
    High-pressure cells for inelastic neutron scattering studies of proton dynamics in materials
12. **Paweł Jochym**
    Not so giant anharmonicity in PbTe
13. **Paweł Karbowniczek**
    Phase behaviour of banana-shaped molecules confined between walls
14. **Łukasz Kolek**
    Molecular dynamics in the antiferroelectric liquid crystal (2S)-octano-2-yl4'-(2-fluoro-4-{[5-(1,1,2,2,3,3,3 heptafluoropropoxy)pentylo]oxy}benzoyloxy)-[1,1'-biphenyl]-4-carboxylate

15. Izabela Łukaszewska

Applications of colorants in OLEDs and photovoltaics

16. Artur Maciąg

Measurement efficiency of Second Harmonic Generation (SHG)
with consideration reflected signals

17 Klaudiusz Majchrowski

Quantum Entanglement in Double Quantum Well-,
Double Quantum Wire -Structures and Jaynes-Cummings Model

18. Klaudia Mencel

Formamidinium Iodide: insight into thermal,
electrical and spectroscopic properties

19. Grzegorz Pająk

Heliconical and other modulated nematic liquid crystals
within Landau–de Gennes description

20. Maria Podgórna

Raman scattering investigations of phase transitions
in the nanocrystals of PbZrO3-BiFeO3 system

21. Andrzej Ptok

Magnetic Lifshitz transition in multi-band iron-based superconductors

22. Ivan Rychetský

Permittivity of polycrystal – laminar structure

23. Maxim Savinov

Comparative broadband dielectric spectroscopy studies
of relaxor and non-relaxor PbFe1/2Ta1/2O3 ceramics

24. Marek Schomber

The phonon density of states and magnetic properties
of bis-2-phenylethylamine-CuCl4, -MnCl4 and their mixed crystals

25. Wilfried Schranz

Domain wall symmetry is described by layer groups

26. Steffen Schwesig

Magnons in the multiferroic phase of cupric oxide

27. Viktor Soprunyuk

Dynamical properties of supercooled water in nanopores

28. Anna Szeremeta

Electric current relaxation processes in non-homogeneous
bismuth manganite - lead titanate ceramics induced
by annealing in gaseous nitrogen

29. Zita Tokarová

Magnetostructural correlations in copper cubanes

30. Mariusz Trybus

Dynamic stimulation of phase transition
in Triglycine Sulphate single crystals

31. Vitalii Turchenko

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List of posters

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Temperature dependence of the EMR spectra for Ni50-xCoxMn35.5In14.5 Heusler alloys obtained by melt-spinning process

33. Martyna Wojciechowska

Structural and dielectric characterization of haloantimonates(III) and halobismuthates(III) based on diisopropylammonium cations

34. Sławomir Wolski

Electron energy spectrum in 2D quantum dot

35. Fabian Ziegler

Multiferroic Hübnerite with unusual high molybdenum doping studied by x-ray powder diffraction and Raman spectroscopy

36. Paweł Zięba

New composite gyrotropic metamaterial

37. Paweł Zięba

Zitterbewegung and symmetry switching in the Klein's four-group

Video lecture to be presented during poster sessions

Lantham Boyle

Choreographic crystals

ABSTRACTS

Sunday 27 VIII

Sunday 27 VIII – Opening Lecture

Many-particle physics: From Smoluchowski to the quantum strongly correlated matter

J. Spałek

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Marian Smoluchowski was the main disciple of Ludwig Boltzmann and contributed in an essential manner to the development of classical statistical physics. Among his achievements is the formulation of the theory of Brownian motion, now known as the Einstein-Smoluchowski theory of kinetic phenomena of many-particle systems. He died prematurely at the age of 45 in 1917. In the first part of my talk I characterize briefly the scientific background of the times and Smoluchowski's Göttingen lectures (1913) introducing, among others, the statistical irreversibility.

In the second half I jump to the contemporary considerations of quantum strongly correlated systems such as the high-temperature superconductors and those exhibiting the Mott-Hubbard localization-delocalization transition. I emphasize the selected statistical properties of those many-particle assemblies and underline the features, by which they differ from the systems of weakly or noninteracting particles considered in textbooks on statistical physics. In particular, I discuss a concrete example of how the statistical ensemble of quantum indistinguishable particles may turn into that of partly distinguishable, albeit not classical particles.

The talk will be of a general character, mainly concerned with specific physical phenomena rather than with the mathematical details.

The research was partly supported by the Grant MAESTRO, No DEC-2012/04/A/ST3/00342 from the National Science Centre (NCN) of Poland.

ABSTRACTS

Monday 28 VIII

Monday 28 VIII - Invited Lecture

Modern approaches probing phonons with X-rays: Magneto-elastic waves in quantum magnets and the full elasticity tensor from thermal diffuse scattering

B. Wehinger

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Inelastic X-ray scattering (IXS) with meV energy resolution is an ideal tool to study lattice vibrations in crystals. IXS can be also sensitive to other degrees of freedom if strongly coupled to the phonons. One intriguing possibility is when polar phonons couple to spin waves in an ordered magnet. This creates electromagnons, quasiparticles that possess both magnetic and electric dipole moments. In this presentation, I will show, that the strong magnon–phonon coupling in the triangular quantum magnet $LiCrO_2$ enables the measurement of magnetic correlations throughout the Brillouin zone via IXS [1]. Our study reveals intricate details of the magnetoelastic excitation spectrum. We found single particle excitations with momentum dependent lifetime and continuum scattering at low temperature. Moreover, we observed over-damped modes, para-electromagnons, above the Néel temperature.

The second part of my talk focuses on the quantitative analysis of thermal diffuse x-ray scattering (TDS). I will show that high-precision measurements of diffuse scattering intensities together with a rigorous data analysis allow the determination of the full elasticity tensor in a single crystal diffraction experiment [2]. Our approach enables a reliable and model-free determination of the elastic properties and can be performed together with crystal structure investigation in the same experiment.

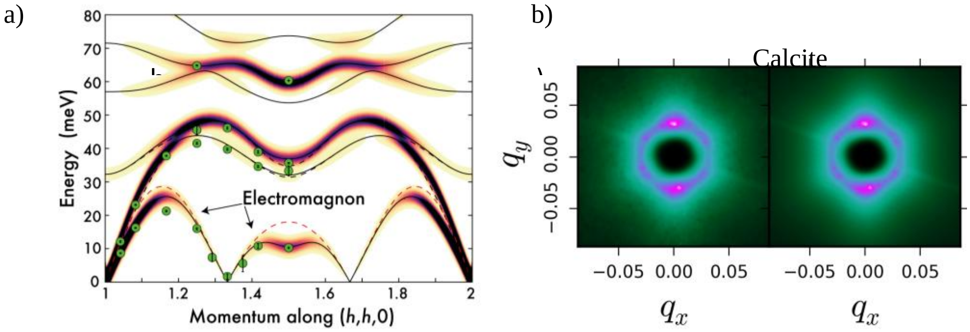

Figure 1. a) Phonon and electromagnon dispersion in $LiCrO_2$ measured by IXS. b) TDS in Calcite, measurement (left) and fit (right) for the determination of the full elasticity tensor.

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Monday 28 VIII - Invited Lecture

DFT meets Landau: A finite strain Landau theory of high pressure phase transitions

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Landau theory (LT) continues to represent an cornerstone of the theory of structural phase transitions. On the other hand, the last decades have seen a tremendous success of ab initio methods in condensed matter physics. In particular, density functional theory (DFT) calculations are nowadays indispensable in analyzing phase transitions at high pressure. Yet, the concepts of DFT and LT are to some extent antipodal. Indeed, condensed matter broken symmetry phases usually appear at low temperature and are thus accessible by ab-initio methods. In contrast, the high symmetry reference phase, which is the pivotal reference frame of LT, only exists at elevated temperatures. On the other hand, while imposing high pressure usually does not pose serious additional difficulties in DFT, an attempt to similarly extend LT to include high pressure phase transitions that involve nonlinear elasticity as a central ingredient turns out to be a non-trivial enterprise. DFT and LT thus appear as complimentary concepts, and the question of how to blend these two approaches in an efficient way continues to be an active area of research.

Recently we have succeeded in constructing a DFT-guided extension of LT to high pressure [1]. Essential for the success of this approach is the ab initio calculation of pressure-dependent elastic constants. Its practical applicability as well as the increase in numerical precision over a standard Landau description are demonstrated by discussing its application to the cubic-tetragonal high pressure phase transitions of SrTiO3 [1], PbTiO3 [2] at ambient temperature and some new results on KMnF3. In addition, a new symmetry-adapted version of the formalism is presented that should finally provide the structural simplicity and transparency required for a widespread use of our theory among the structural phase transition community.

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Monday 28 VIII

Mass-resolved neutron spectroscopy

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Neutron Compton scattering (NCS) is a unique experimental technique made possible by the development of epithermal neutron sources, such as the ISIS source of the Rutherford Appleton Laboratory in the UK [1, 2]. The measurement of nuclear momenta by high-energy neutron Compton scattering relies on the fact that the energy and momentum transferred in the scattering process are sufficiently large, such that the so-called impulse approximation (IA) is an accurate starting point. In the IA limit, the dynamic structure factor measured in NCS for a given nucleus is determined by the nuclear momentum distribution (NMD). In the picture of purely classical nuclei, the NMD shape is determined by whole energy spectrum of the motional modes, including translational and rotational modes, followed by lattice and internal molecular vibrations. However, more and more experimental evidence has been accumulated over the years that nuclear quantum effects, with nuclear zero point motion being the most prominent, also contribute to the NMDs. Since its birth, the NCS technique has been employed to study proton momentum distributions in quantum fluids and solids, metal hydrides and gas and charge-storage media, etc. Beyond the proton, recent instrument developments towards MANSE (Mass-resolved Neutron Spectroscopy) offer the prospects of access to the NMDs of heavier nuclides including deuterium, helium, lithium, carbon, oxygen, and fluorine. I will present some examples of recent MANSE work advocating the use of a combination of ab initio tools and neutron scattering techniques for the characterisation of nuclear chemical dynamics in the solid state with the special emphasis on hydrogen bonded molecular crystals (see [3] and Fig 1).

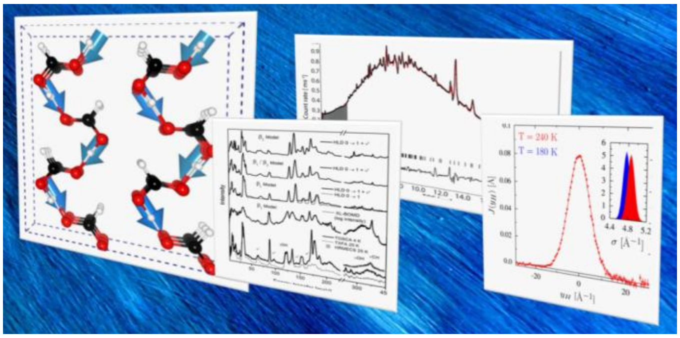

Fig. 1. Neutron Compton Scattering applied concurrently with inelastic neutron scattering and neutron diffraction and augmented with DFT calculations (adopted from [3]).

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Monday 28 VIII

Alternative approaches to zeros and poles of dielectric function – beyond the harmonic phonons

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Infrared spectroscopy and broad-band dielectric spectroscopy has been traditionally employed to study lattice dynamics of highly polarizable solids and in particular, the pre-transitional lattice dynamics of crystals with ferroelectric and other related structural phase transitions. Very often it turned out that the number of the Brillouin zone centre modes expected from the linear response theory or the group analysis does not correspond to the number of independent damped harmonic oscillators needed to describe satisfactorily the dielectric function of such materials. Typically, in these cases one has to introduce either some extraneous excitations or to employ a more generalized phenomenological model, going beyond the straightforward superposition of damped harmonic oscillator response functions.

The aim of this contribution is to review various such phenomenological models, used to describe anharmonic lattice dynamics, and to formulate a systematic strategy permitting their direct comparisons. Proposed procedure will be explained in simple terms and illustrated on various numerical examples ranging from the soft modes of the classical ferroelectric perovskites to the recently studied families of multiferroic materials as for example the lacunar spinels of GaV4S8 family.

Monday 28 VIII

Raman and IR-active coupled modes in GaV4S8

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Recently, GaV4S8 has attracted a lot of attention due to the fact that this crystal can host so-called skyrmion agnetic phases [1,2]. However, the material is interesting also as a prototype ferroelectric material with non-centrosymmetric paraelectric phase where the ferroelectric phase is induced by the Jahn-Teller transition [3]. Since the paraelectric soft mode of this structure is simultaneously Raman and IR active, in principle, both Raman scattering and IR reflectivity can reveal soft mode dynamics. However, since the transition is of the order-disorder type, the Cochran-like soft-mode behaviour is not present [3]. Nevertheless, the overdamped mode corresponding to the frozen polar distortion seems to show considerable damping and peculiar lineshape anomaly, related to the mode-interference phenomenon [3]. In this work, the Raman spectra of GaV4S8 ceramics are thoroughly analyzed by the response of coupled damped harmonic oscillators and the resulting model is confronted with the infrared reflectivity spectra of the same material.

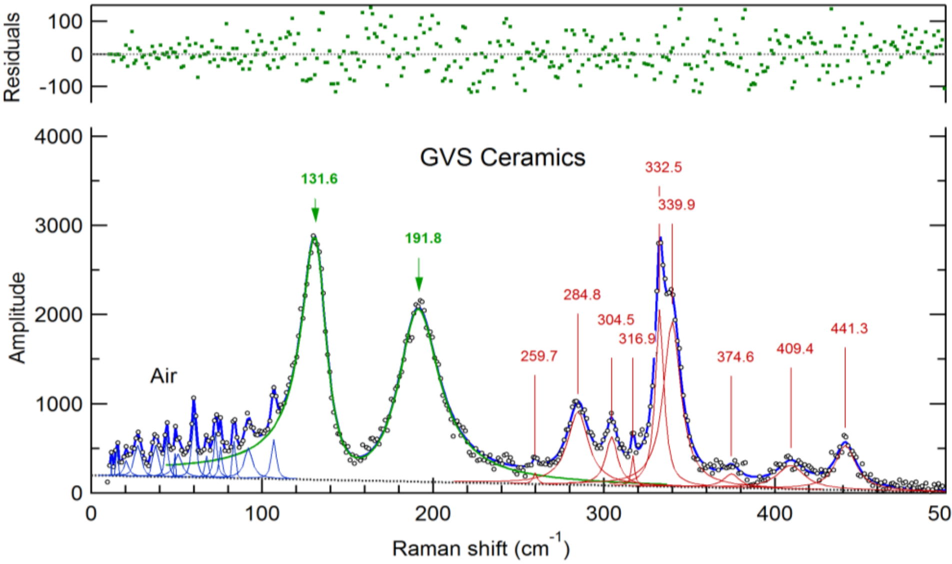

Fig. 1. Room temperature Raman spectra of GaV4S8 ceramics. Raman bands are fitted with harmonic oscillators (red). The two strong Raman bands located in the 100-230 cm-1 range comply with the model of coupled damped harmonic oscillators (green). Note: Weak narrow lines (blue) below ~120 cm-1 come from rotational Raman transitions of N2 and O2 molecules in the surrounding air.

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Phonons from neutron diffraction

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Neutron diffraction was one of the first techniques to determine phonon dispersion curves before inelastic spectroscopy became routine. Initially, dispersion curves were determined along high-symmetry directions in rather simple compounds [1]. Generally, phonons manifest themselves in the form of thermal diffuse scattering in a diffraction experiment. The thermal diffuse scattering is integrated in energy but resolved in momentum. A peculiar effect is observed in time-of-flight single crystal neutron diffraction on a pulsed neutron source using many incident wavelengths simultaneously. In this case, neutrons can accidentally match the energy and momentum and direct phonon excitation can occur [2]. This leads to thermal diffuse scattering that breaks the symmetry of the diffraction pattern. It was not until recently, that this effect could be simulated using a novel approach combined with density functional theory calculations [3]. The methodology will be discussed and results from recent experiments and simulations will be presented.

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Monday 28 VIII – Invited Lecture

Dielectric relaxation processes in glassy and liquid water

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Water exhibits a plethora of fascinating anomalies and continues to generate numerous controversies. Among them is the existence of different metastable states at low temperatures, namely the low-density and the high-density amorphous ices [1]. In this contribution we will present the dielectric responses of these two states [2]. Based on recent experimental findings we will discuss whether their underlying dynamics reflects truly structural fluctuations or merely proton motion as in crystalline ices [3]. Additionally, we will focus on the kinetics of the transitions between the two amorphous states, and on the role played by quantum effects for the dynamics of ultracold water [4]. Regarding the other side of its "no man's land", several recent studies revisited the relaxation behavior of water above its melting point [5]. Here research is stimulated by the progress in understanding gained from the investigation of monohydroxy alcohols. In this respect we performed a detailed comparative analysis which allowed us to clearly identify the dielectric signature of the relaxation process in water [6]. Our findings vindicate the apparent inconsistency between the dielectric and rheological properties of this peculiar liquid and shed new light not only on the microscopic origin of its anomalously large polarization exploited in microwave heating but also on the conflicting debate regarding dynamics in amorphous ices.

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Monday 28 VIII

Influence of doping on the absorption of hydrogen in AB_5 – type intermetallic compounds

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Hydrogen belongs to the most environmentally friendly fuels which can be obtained in different ways. The most efficient and, currently, the dominant technology of H_2 production is hydrocarbons steam reforming. Some alternative methods are based on electrolysis, thermolysis or microbial biomass conversion. The latter approach is considered to be one of the most attractive alternative biological methods of hydrogen production. In fermentation-based systems, microorganisms, such as bacteria, break down organic matter to produce biohydrogen. The organic matter can be sugar beet molasses, green biomass, and even municipal waste. Hydrogen/biohydrogen can be stored using methods like: cryogenic tanks (liquid hydrogen), high-pressure gas cylinders, absorption on materials with a large specific surface area, chemical bond in ionic and covalent compounds, or absorption on interstitial sites in a host metal. In the latter case the metallic hydrides of intermetallic compounds are especially interesting. To their advantages belong high efficiency of sorption/desorption processes and acceptable temperatures/pressures for mobile applications. A typical representative of this group is $LaNi_5$. Dopants can influence hydrogen absorption in this compound. Several transition metal dopants of $LaNi_5$ were selected on the basis of DFT computer simulation, and next the samples were prepared. Only dopants substituting nickel at concentration below 20% were considered. The kinetics of hydrogenation and dehydrogenation improves according to expectations. Particularly, the dopant element Ag shows a quite significant reduction in equilibrium pressure (compared to $LaNi_5$) while dopants Bi, Fe, or Si degrade the hydrogen storage capacity. Structural and thermodynamic (*cpT*) results will be presented and discussed.

Acknowledgement:

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A unified mechanism of dielectric relaxation in water and ice

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Water ice shows an extremely high self-diffusion coefficient for crystals [1]. During the Debye relaxation time (~ 0.2 ms) the labeled oxygen atom travels to a distance of 8-9 molecule dimensions. Current view implies intensive microscopic transfers in ice but only occurring in the proton subsystem. It is believed that there exists a migration of defects in the hydrogen bond structure responsible for the high dielectric constant of ice. A particular mechanism of dielectric relaxation and conductivity both in water and ice is still controversial.

In this talk we expand our radically new understanding of water structure dynamics on ice [2-4]. We analyse comparatively the dispersion features of the broadband dielectric spectra of water and ice (Fig.1) to develop a unified model of the atom-molecular diffusion. The dynamics of the structure is considered as a process of creation/destruction of H3O+ and OH- ions. The particles thus born migrate for a time through thermal collisions. Each ion transforms into a neutral H2O molecule and reversely an H2O molecule transforms into an ion. The H2O molecules and counterions H3O+ and OH- are in thermal equilibrium. According to the model, both water and ice possess a huge amount of short-living counter ions (~ 1M) the dynamics of which exhaustively determines their electrodynamic response.

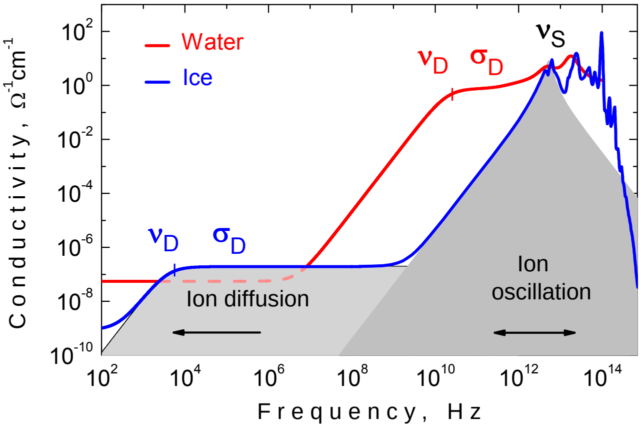

Fig. 1. Broadband conductivity spectra of water and ice at ~ -10 C (red and blue). The diffusion plateaus σD and frequencies νD represent the Debye relaxation filled by charges from the νS-oscillator.

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Monday 28 VIII

Langevin dynamics and sedimentation of nanoparticles

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The Brownian motion and diffusive type of transport are fundamental for understanding many phenomena across different areas of science and technology. In this vast research area, interesting new analytical results of fundamental importance have been obtained quite recently [1]. Nevertheless, a great deal of open questions still remain to be answered [1].

Our goal is to discuss a theoretical description of nanoparticles in the suspension and in the presence of the external field. In particular, we would like to consider Langevin dynamics of particles in fluids under influence of the gravitation force. The Langevin approach to nanoparticles in suspension has been pursued by many theoretical studies (see eg. [2,3]). In our modelling of sedimentation and possible mechanisms of nanoparticle aggregation we will try to include applied methods underlying recent numerical simulations [2,3] and ideas following from a new theory of Langevin dynamics with spatially correlated noise [1].

Gravitational sedimentation could be also investigated experimentally with submicron or nanoparticles of hematite in various water solutions (see eg. [4]). Using the Mössbauer spectroscopy one can obtain velocity profiles of the particles at different positions (depths) of the solution [4]. The experimental data can therefore provide some validation of our theoretical model. The comparison of our theoretical approach with experimental results, where available, may provide important clues regarding both the fundamental open questions and applications.

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Monday 28 VIII

Ionic conductivity in Metal-*closo*-Borates

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Solid state compounds with ionic conductivity larger than 1 mS/cm at room temperature can compete with liquid electrolytes when applied in rechargeable batteries. Recently new such materials were discovered, extending family of ionic conductors based on oxides and sulfides.

Another new class of new fast ionic conductors was found within borohydride family, as a by-product of hydrogen storage research. Especially, very high conductivity of sodium reported in $Na_2B_{12}H_{12}$ competes with the best solid state conductors known for this metal. Further developments brought borane based Na superionic conductors that are by orders of magnitude better than those based on β-alumina.

The origin of cation mobility in this class of materials remains still puzzled. We will present examples of theoretical studies, based on DFT calculations, covering problems related to structure, dynamics, and the ionic conductivity mechanism in compounds with BH_4^- and $B_{12}H_{12}^{2-}$ anions. The relation between the superionic conductivity and the crystal structure will be presented in detail [1,2].

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Monday 28 VIII

Dynamical properties of *closo*-Boranes

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In recent years, borane compounds have been studied as ion-conductors for batteries and in various other energy applications. Even though their phonon density of states (DOS) can be measured with various experimental techniques, the computational methods for the correct calculation/estimation of the DOS, have yet to be investigated. In this work, we focus on structures containing the *closo*-borane anion $B_{12}H_{12}^{2-}$ and various metals M (M=Na, Li, Mg). The thermodynamical and structural properties of these compounds are investigated for various approximations of the Density Functional Theory. We show that the incorporation of van der Waals forces is essential for the proper description of their static properties. Furthermore, the dynamical properties of these compounds are calculated. We analyse the performance of selected methods on vibration spectra and compare with available experimental results. The relation between vibrational properties and ion transport will be presented.

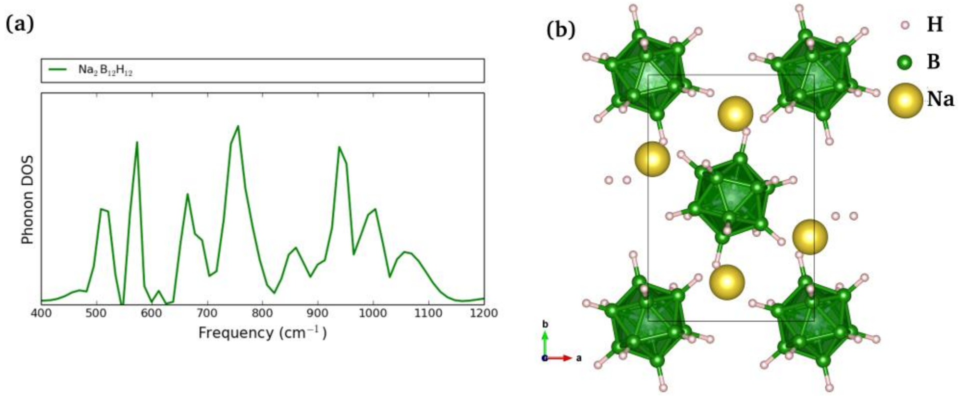

Fig. 1. (a) Phonon Density of States for $Na_2B_{12}H_{12}$, (b) Unit cell structure of the low temperature phase $Na_2B_{12}H_{12}$

Financial support of Swiss National Science Foundation within the Sinergia project ‘Novel ionic conductors’ under contract number CRSII2_160749/1 is kindly acknowledged.

Electric relaxations in nitrogen-doped bismuth manganite ceramics

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The 0.96Bi-Mn-O–0.04$PbTiO_3$ (BM-PT) ceramics was sintered from non-polar bismuth manganite and ferroelectric lead titanate components at 1170 K and ambient air pressure. The ceramics were annealed in nitrogen N_2 flow at 1100 K [1, 2]. The ceramics consisted of three phases: orthorhombic *Pbmn*, sillenite cubic *I23*, and tetragonal *P4mm* in accordance to the X-ray diffraction patterns analysis [2, 3, 4]. Non-homogeneous chemical composition was determined using the SEM tests. The electric impedance, which was measured in frequency f = 200 Hz – 1 MHz and T = 100–650 K ranges, exhibited marked dispersion. The BM-PT ceramics showed two electric conductivity relaxations. One process shown characteristic time value $\tau_{01} \approx 10^{-12}$ s and activation energy E_{A1} = 0.17 eV. Next process shown $\tau_{02} \approx 10^{-13}$ s and E_{A2} = 0.35 eV. Third relaxation processes occurred in the samples BM-PT-N annealed in gaseous nitrogen. This nitrogen annealing induced process exhibited $\tau_{03} \approx 10^{-12}$ s [2, 5]. The influence of the annealing in nitrogen on the resistive switching was tested. The DC resistivity ρ_{dc} temperature dependence showed thermally activated dependence in 400-750 K range. The variable range hopping of small polaron model was fitted for T < 380 K. This feature was consistent with the structural and chemical disorder. The annealing in nitrogen induced increase in ρ_{DC}, by one order in value [2, 3, 5].

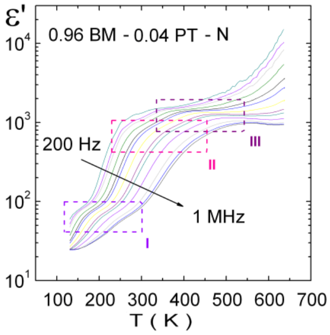

Fig. 1. Real part of the permittivity, ε'(T), obtained for BM–PTO–N ceramics.

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Monday 28 VIII

Inelastic X-ray scattering study of the electron-phonon anomalies in $Nd_{2-x}Ce_xCuO_4$

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Understanding the charge-ordering tendencies exhibited by the cuprates might give valuable insight into the origin of the superconductivity of these complex oxides. Therefore, hard X – ray [1] and resonance soft X-ray [2,3,4] studies, which demonstrated the existence of charge density wave order (CDW) as a universal characteristic of a underdoped cuprates, triggered a tremendous amount of scientific activity. The charge correlations appear to manifest themselves as an anomalous dispersion (softening) of the longitudinal Cu-O bond-stretching phonon mode in the hole-doped cuprates [5,6] and in electron-doped $Nd_{2-x}Ce_xCuO_4$ (NCCO) [7], as indicated by inelastic X-ray scattering (IXS) studies. Although the CDW and phonon softening anomalies were found at approximately the same two-dimensional wave vector (H,K) ≈ (0.2,0) in NCCO, they were studied only up to 380 K and below room temperature, respectively. Here, we report on our recent effort to extend the IXS measurement of the phonon anomaly to higher temperatures, where the CDW order should be relatively weak or absent, in order to seek some indication of a phonon change associated with diminished CDW order.

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Temperature dependence of the EMR spectra for $Ni_{50-x}Co_xMn_{35.5}In_{14.5}$ Heusler alloys obtained by melt-spinning process

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Ni-Mn-In and Ni-Co-Mn-In belong to metamagnetic Ni-Co-Mn-X (X = In, Sn, Sb) Heusler alloys family and shown many promising physical properties, e.g. giant invers magnetocaloric effect, which can be applied in ecological refrigeration. Some properties of these materials, e.g. temperature of martensite transition, could be tuned by appropriate choice of chemical composition of the alloy. One of the problems with application of Ni-Mn-In in industry is its brittleness. The addition of Co reduces brittleness and improves plasticity. Additionally, an increase of Co content up to 5 % at. changes temperature of matrensite transition and shift Curie temperature into the higher region.

In this research we registered electron magnetic resonance (EMR) spectra of off-stoichiometric $Ni_{50}Mn_{35.5}In_{14.5}$ and $Ni_{45}Co_5Mn_{35.5}In_{14.5}$ ribbons which were obtained by melt-spinning process. Temperature dependences of the EMR spectra was recorded in the temperature range 180-300 K.

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Monday 28 VIII

Synthesis of narrow band gap perovskite Ba(Zn,Ti)O_3 ferroelectric thin films for environmental friendly photovoltaic conversion

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A novel generation of photovoltaic and optoelectronic devices based on ferroelectric perovskites take advantage of the poled electric field through the material in order to direct the photo-generated charges (electron-hole pair) to the respective cathode-anode, hence improving conversion by preventing recombination and avoiding the energy barrier of junctions architecture. Nevertheless, most conventional perovskite oxides usually have relatively wide band gap (>2 eV) and hence small PV efficiencies; whereas organic-inorganic Pb-halide perovskites still face issues towards commercialization due to the need to achieve fabrication reliability, long-term stability and the employ of potential toxic elements [1]. In this work the structural, optical and ferroelectric properties of the Ba($Zn_{0.5}Ti_{0.5}$)O_3 thin films grown on Pt/TiO_2/SiO_2/Si substrates by rf-sputtering are evaluated. This novel perovskite-like oxide material has a low band gap of 1.48 eV and exhibits polarization properties which can signify a real potential for application in the harvesting of optical energy.

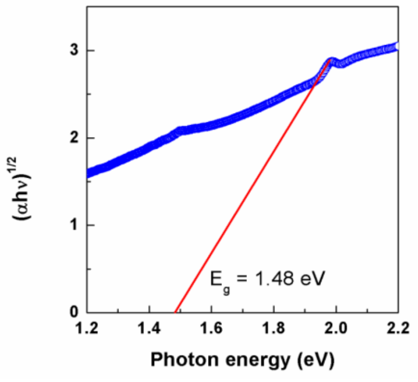

Fig. 1:($\alpha h\nu$)$^{1/2}$ versus incident photon energy plots for Bi($Zn_{1/2}Ti_{1/2}$)O_3 thin films. Optical band gaps were determined via the linear extrapolation in Tauc method.

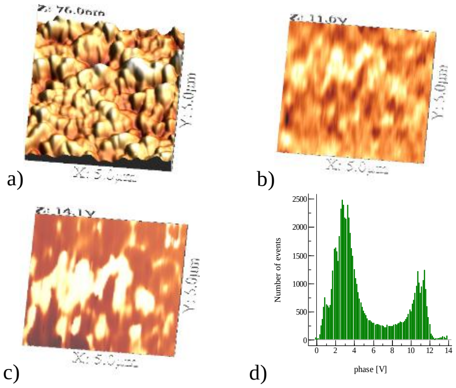

Fig. 2:PFM scans of BZT thin film sample surface a) topography, b) amplitude, c) phase and d) respective histogram [2].

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Suppressed electron-phonon coupling due to strong spin-orbit interaction at the Tl/Si(111) surface

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We study the effect exerted by the electron spin and the spin-orbit coupling on the remarkably strong electron-phonon interaction found at the Tl/Si(111) surface. The particular spin texture of this surface governs the whole low-energy electron-phonon dynamics, which are specially characterized by the overlap of initial and final electron spin states. We show that the electron-phonon coupling strength is strongly modulated for surface states in the vicinities of the Γ point, and even almost suppressed close to the K point valleys. The lowest energy longitudinal surface phonon mode is hardened by a factor of two as a result of the presence of the electron spin. Our first principles results are qualitatively supported by a simple model of the electron-phonon matrix elements including spinor states.

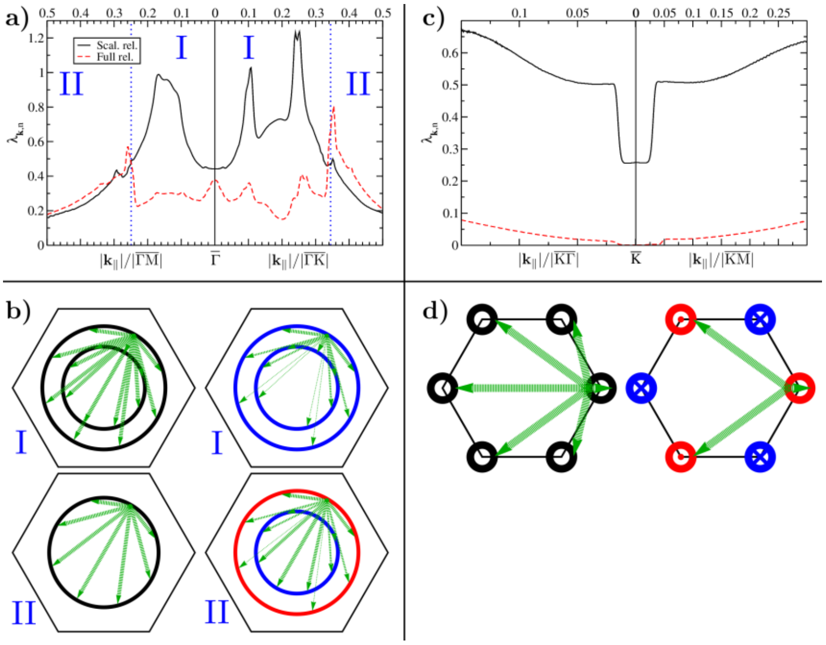

Fig. 1. Dependence of the el-ph interaction λ parameter on the momentum k. The scalar and fully relativistic cases are represented by solid (black) and dashed (red) lines, respectively. (a) λ_k along the highest energy occupied surface band close to Γ point. (b) Fermi contours and scattering processes without (right) and with (left) electron spin for states close to Γ point. (c) λ_k along the lowest energy unoccupied surface band close to K point. (d) Fermi contours and scattering processes without

Monday 28 VIII

Beam-induced atomic motion in oxide glasses

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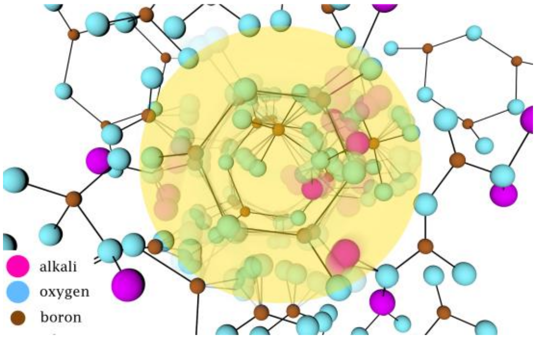
Powerful X-ray sources with a high brilliance are considered as ultimate tools for probing microscopic properties in materials. In the case of soft materials as polymers or biological samples it is well known that the beam is not only probing but at the same time modifying the structure and the dynamics of the irradiated part of the sample causing chemical rearrangements up to complete disruptions. In hard-condensed matter, however, X-rays also affect the system mainly through radiolysis, knock-on events or electron rearrangements. Hence, being aware of the dynamical and the structural influence due to the beam (see figure) is crucial for determining the actual intrinsic properties of such materials.



Beam-induced dynamics in alkali borate glass: Pumping and probing at the same time

By collecting series of diffuse scattering patterns with coherent X-rays, aXPCS becomes a very powerful technique of probing the atomic motion in crystalline and amorphous materials. The resulting “movie” of speckles provides information of the atomic dynamics like the decay time τ and the diffusion constant D dependent on the sample itself, the scattering vector q and the temperature. So far, the unawareness of the measured dynamics triggered by the X-ray beam at aXPCS experiments leads to misinterpretations of τ and D. Ruta et al. [1] were able to show that in vitreous SiO_2 and GeO_2 τ is inversely proportional to the flux of the beam. Moreover, she shows that at fixed flux the dynamic remains stationary and is q-independent. We extended the “pump and probe” investigations to different kinds of borate and silicate glasses, lead silicates [2] and vanadium phosphate glasses, finding out that the effect varies from sample to sample and is, in contrast to our expectations, not disappearing when measuring the sample close to the glass transition temperature. Furthermore, the “pump and probe” effect could be seen as a great opportunity to indirectly probe physical properties of materials like bonding properties.

The work was funded by the Austrian Science Fund (FWF): P28232-N36.

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Lattice dynamics of a quasi-2D layered TlCo2Se2 with a helical magnetic structure

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The dynamical properties of a quasi-two-dimensional layered TlCo2Se2 compound exhibiting an incommensurate helical magnetic order [1] were investigated within approximation of the harmonic phonons and using the density functional theory (DFT). The helical magnetic structure of this ternary dichalcogenide was shown to be stabilized by phonons. The calculations have shown that the intensities of the Raman and infrared active phonon modes of TlCo2Se2 remained sensitive to magnetic interactions, which are quite strong within the Co–Se layers [2]. Results of our investigations allow to clarify the origin of substantial differences between dynamical properties of TlCo2Se2 with helical magnetic structure, ferromagnetic KCo2Se2 [3], and the Pauli paramagnet KNi2Se2 [4].

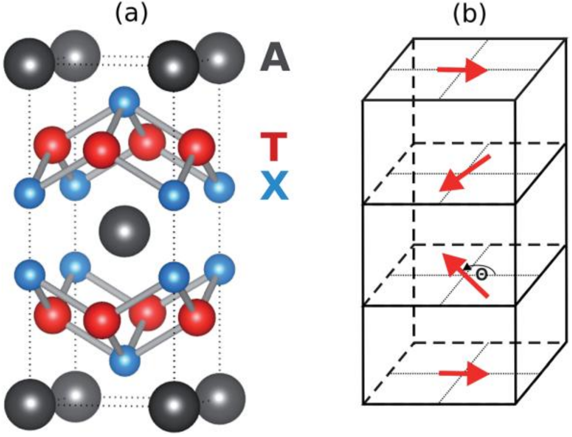

Fig. 1. (a) Tetragonal structure of the AT2X2 compounds (space group I4/mmm, no. 139). Wyckoff positions: A (2a), T (4d), and X (4e). (b) Schematic of the TlCo2Se2 magnetic helix with a turn angle Θ ~ 121° running along the crystal c-axis.

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Monday 28 VIII

Confined lattice dynamics in ultrathin Ge/Fe3Si/GaAs heterostructures

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Reducing the dimensions of devices to the nano- and subnanometer scale leads to alteration of almost all properties that could either enhance or deteriorate their performance. It has already been demonstrated that the finite dimensions at the nano length scale significantly modify the thermal lattice excitations [1]. The phonons become more pronounced and complex, and play an important role for heat dissipation, thermal management, and 1/f noise of the nanodevices, influencing their thermal stability, lifetime, and performance [2]. Therefore, for both the fundamental research and nanotechnological applications the comprehensive understanding of the confinement effects on the thermoelastic properties of nanomaterials is of paramount importance.

We studied the phonon properties of ultrathin 57Fe3Si layers in Ge/57Fe3Si/GaAs heterostructures as a model system for lattice dynamics modifications in metal/semiconductor interfaces. Epitaxial 57Fe3Si layers with thicknesses from 2ML to 36ML (1ML = 0.28 nm) were grown on GaAs(001) substrates [3] and capped by a 4 nm thick amorphous Ge layer to prevent the alloy from oxidation. In situ electron diffraction measurements showed the formation of smooth Fe3Si films at a layer thickness of 3ML, while X-ray diffraction and reflectivity measurements revealed a perfect stoichiometry and high interface quality. Nuclear forward scattering (NFS) and nuclear inelastic scattering (NIS) experiments were performed at P01, PETRA III at DESY. The NFS results showed that the ferromagnetism is lost between 6 and 3 ML Fe3Si film thickness; that is in agreement with earlier studies [4]. NIS was used to determine the iron-partial phonon density of states at room temperature as a function of the interface layer thickness. While the phonon DOS of the 36 ML sample is fully reproduced by the ab initio calculated DOS of bulk Fe3Si, significant deviations are observed for lower interface thicknesses leading to anomalies in the thermoelastic properties of this alloy.

This work is financed by the Initiative and Networking Funds of the President of the Helmholtz Association and the Karlsruhe Institute of Technology (KIT) (contract VH-NG-625) and the Federal Ministry of Education and Research BMBF via the Verbundprojekt NUKFER (contract 05K16VK4).

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Monday 28 VIII

High stability of magnetite thin films under high-energy ion irradiation

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Magnetite (Fe_3O_4) - the oldest known magnetic material has been studied since the early days of science. Since the 1960s magnetite has been investigated extensively due to its high potential for technological applications in many important fields, e.g. high-density recording media and catalysis. During the last few decades a re-new attention has been paid to Fe_3O_4 in particular the magnetite films, due to their potential application as spin dependent transport devices.

The physical and structural properties of interfaces play a crucial role in obtaining well-orientated thin films. It is important to point out here that while a large effort is focusing on the magnetite film surface properties and terminations, their interfaces have been less studied and there is a lack of the knowledge of interdifussion and intermixing effects and the film stability in the external conditions such as annealing and especially high-energy ion irradiations. To the best of our knowledge, there is no report on such a research for Fe_3O4 thin films, except of our publications (for very thin films [1] and for thicker films (recent work)). There existed some reports devoted to using the swift heavy ions to modify the magnetic and transport properties of magnetite films.

We have investigated both the single- and bi-layer Fe_3O_4 films prepared by a Molecular Beam Epitaxy (MBE) technique on MgO(001) substrates (Fe_3O_4/MgO(001) and Fe_3O_4/Fe/MgO(001)). To study the interdiffusion, selected films have been treated by a subsequent annealing, while for ion-beam mixing study, the films have been irradiated by the 1MeV Ar^+ and Kr^+ ions with different ion fluences in the range of 10^{15} - 10^{16} ions/cm^2. The film crystallinity, composition and layer thicknesses have been characterized by the X-ray reflectometry (XRR), Rutherford back-scattering (RBS) and RBS-Channeling (RBS-C).

Our results confirm that the stoichiometric Fe_3O_4 surface layer can be always obtained for Fe_3O_4/Fe/MgO(001) films. Such a layer was remained stable upon thermal annealing as well as in exposing to air, although the large lattice mismatch at both Fe_3O_4/Fe and Fe/MgO interface implies a degradation of the film crystallinity. The bi-layer structure and the stoichiometric Fe_3O_4 layer on the film surface were well preserved after Ar^+ and Kr^+ ion irradiation at low damage levels, although the strong intermixing implied a large interfacial (Fe_xO_y) and (Fe,Mg)O_y layer respective at Fe_3O_4-Fe and Fe-MgO interface. We found e.g. the high ion fluence of 3.84×10^{16} Kr/cm^2 has induced a complete oxidization of the buffer Fe layer, but the stoichiometry of the Fe_3O_4 surface layer was conserved indicating its high stability under Kr^+ ion irradiation.

The magnetite thin films with properly chosen parameters for ion-beam modification experiments were prepared within the scope of cooperation with Prof. J. Korecki (AGH Kraków).

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Composition dependence of selected mechanical properties of (Pb,Cd)Te crystal lattice

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Lead telluride is one of the lead chalcogenides, which are considered very useful on the field of thermoelectricity and infrared detection. In a single PbTe bulk crystal grown by the Bridgman method the microhardness maintains almost a constant value of ~ 30 HV for various carrier concentrations [1]. Due to the relatively low microhardness value a layer of PbTe is so soft that it can be easily scratched. Consequently, some devices consisting of layers of PbTe are not robust enough to withstand the damage possible in a standard fabrication processing [2]. In order to avoid this problem more robust materials are typically chosen as an outermost layer or PbTe is replaced by a solid solution containing some amount of another compound like, e.g., GeTe [2].

The aim of present studies is to demonstrate the crystal lattice hardening resulting from noticeable CdTe content in the (Pb,Cd)Te solid solution. All single (Pb,Cd)Te crystals containing from 0 to 10% of the CdTe were grown at the Institute of Physics PAS by the self-selecting vapor growth (SSVG) method [3]. The room temperature data about microhardness and Young's modulus were determined by the nanoindentation method using an Ultra Nanohardness tester CSM UNHT/AFM and the Berkovich indenter tip. The average values and standard deviations of the hardness and Young's modulus were extracted from the determined load-displacement results. The anisotropy of these parameters was estimated by the nanoindentation for selected samples. The composition-dependent ultrasound velocity was estimated for the same set of solid solutions using the LA phonon dispersion data, obtained by inelastic neutron scattering (INS) measurements. Correlation between composition of investigated crystals and their selected mechanical properties is given and discussed in comparison with the available relevant data for (Pb,Ge)Te solid solution.

This work was supported in part by National Science Centre (Poland) through grant UMO-2014/13/B/ST3/04393.

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Monday 28 VIII

Synchrotron Solaris

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An overview of National Synchrotron Radiation Centre SOLARIS: a short history of the project, main components and parameters of the SOLARIS synchrotron, SOLARIS offer for researchers. The SOLARIS synchrotron is the most modern and largest multidisciplinary research tool in Poland. It outstanding capabilities place it firmly at the cutting edge of devices of this type. As a strategic investment for the development of science, it has been included in the Polish Roadmap for Research Infrastructures. The Centre was built between 2010 and 2015. The investment was co-financed by the European Union with funds from the European Regional Development Fund, as part of the Innovative Economy Operational Programme for 2007-2013.

Monday 28 VIII – Invited Lecture

Tuning dynamic properties of polymer nanocomposites

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Polymer nanocomposites (PNC) play important role in many current technologies due to their light weight, high tunability of properties, and relatively low costs. It is now well recognized that interfacial layer formed around nanoparticles controls macroscopic properties in PNCs. In this talk we overview recent studies on structure and dynamics of the interfacial layer in various polymeric nanocomposite materials. We overview broad array of experimental techniques and MD-simulations that provide detailed characterization of the interfacial layer at the nanometer scale. Dielectric relaxation studies and MD-simulations reveal a gradient in the interfacial layer dynamics [1-3]. Small angle X-ray scattering, dielectric spectroscopy and differential scanning calorimetry provide consistent estimates of the interfacial layer thickness in various PNCs [1,3-5]. The thickness of the layer increases upon cooling to Tg [3], and depends strongly on polymer rigidity [2,6], increasing from ~2nm in flexible polymers to ~5 nm in more rigid ones. At the same time, the increase in stregth of the polymer-nanoparticle interactions does not affect the thickness of the interfacial layer, but increases the slowing down of its dynamics [2]. Detailed studies revealed unexpected molecular weight dependence of PNCs properties ascribed to frustration in packing of long polymer chains in the interfacial region [4]. All these results clearly demonstrate the existence of the interfacial layer with much slower dynamics that propagates a few nm (~2-5 nm) into the polymer matrix, but no signs of any long range (larger than ~10nm) effects. Analysis of mechanical properties using Brilloin light scattering and advanced scanning probe microscopy [5] revealed more than 2 times increase in the glassy polymer modulus in the interfacial layer. This huge increase was ascribed to stretching of the chain in the interfacial region. Analysis of dynamics in PNCs below Tg revealed that fast picosecond fluctuations and secondary relaxation are getting faster in the interfacial layer, in contrast to segmental dynamics that slow down. We ascribe this effect to frustration in chain packing around nanoparticles that leads to lower density and faster local dynamics, while stretching of chains leads to slower segmental dynamics and higher elastic modulus. At the end, we present a general picture how microscopic parameters control the interfacial layer, and how by tuning the interfacial layer we can tune macroscopic properties of polymer nanocomposites.

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Monday 28 VIII

Effects of confinement on molecular dynamics of glass forming-liquids

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This work is motivated by a number of recent studies concerning the impact of confinement on the glass transition. In general, a glass is defined as a disordered material which lacks the crystalline order but has macroscopic properties of solid. A vitreous state can be obtained for both organic and inorganic systems if they are cooled fast enough to avoid crystallization. The understanding of the glass transition phenomenon has great significance for material engendering, as well as for the pharmaceutical and food industries. For applications of many materials, the vitreous state is more favorable than the crystalline phase. One way to influence the phase diagram in this regard is by spatially restricting the substance in nanopores. The effect of confinement on molecular dynamics is usually demonstrated as i) the deviation of structural relaxation from the Vogel-Fulcher-Tammann temperature on approaching the T_g, ii) existence of the slow, additional dynamics processes interpreted as resulting process of molecular interaction with the pore walls, iii) depression of T_g.

In the current contribution, Broadband Dielectric and Fourier-Transform Infrared spectroscopy are combined to study the molecular dynamics of two glass forming liquids: poly(ethyleneglycol) phenyl ether acrylate (PEGPEA), and poly(ethylene glycol) dibenzoate (PEGD), confined in unidirectional nanopores of mean diameters 4, 6 and 8 nm. The *intra*molecular mobility is revealed by analysing the temperature dependencies of positions and intensities of specific IR absorption bands and compared with *inter*molecular dynamics obtained by dielectric measurements. It is shown that intra-molecular dynamics becomes less sensitive to temperature under nanoscale confinement, a finding attributed to changes in the local density of the molecules in nanopores. The impact of pore sizes on motions of particular molecular units is found out. The effect of different end groups i.e. phenyl rings, acrylate functional group on the dynamics of ethylene glycol chains is also elucidated.

Acknowledgements
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Monday 28 VIII

Complementary study of solid state polymorphism in ethosuximide

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Ethosuximide (2-ethyl-2-methylsuccinimide) is used in the treatment of epilepsy [1]. One can find in literature the publications about its bioactivity studies [1-2]. There are also multiple reports about its analytic studies, which yields the information how to determine qualitatively and quantitatively the ethosuximide in mixture drugs [3]. There is no information about ethosuximide polymorphism and physico-chemical properties. Therefore to establish polymorphism of ethosuximide we used many complementary methods: polarizing microscope observation, X-ray diffraction, dielectric spectroscopy and infrared spectroscopy. The study shows that ethusuximide is a good glass former as the existence of two CONDIS crystals was observed. The investigation shows the influence of details of molecular structure and dynamics and interactions between molecules on the sequence of phase transitions.

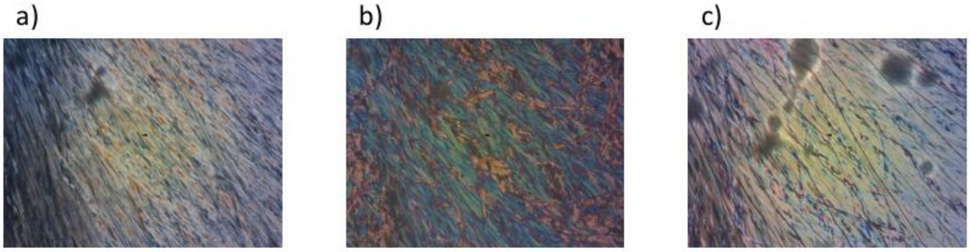

Fig. 1. Textures of ethosuximide phases observed during cooling with rate of 10^0/min: a) CONDIS Cr_1 (48^0C), b) CONDIS Cr_2 (25^0C) and c) glass of CONDIS Cr_2 (-30^0C).

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Monday 28 VIII

Thermodynamic and dynamic properties of glass of disordered phases

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We present results of complementary measurements for selected glass-forming soft mater compounds. There are several features that characterise a glass of a disordered phase [1], i.e. the one lacking long-range order, such as: jump of the heat capacity, relaxation of enthalpy, presence of the boson peak, residual enthalpy responsible for disorder of spatial distribution of molecules, appearing or disappearing of cracks on textures observed under a polarizing microscope, broadening of FT-IR absorption bands and of X-ray diffraction peaks, an excess of vibrational density of states unveiling during vitrification and softening of glass. Upon softening, glasses of a plastic-crystal phase or of liquid crystal mesophases, arrive at metastable states which, during further heating, undergo a 'cold crystallization' (recrystallization) to a more ordered crystal phase with long-range and local interactions between molecules. This transition is, in fact, a two-stage phenomenon: (i) nucleation and (ii) growth of crystallites of the new phase [2,3].

It has been proved that hydrogen bonding plays an essential role in the forming of glass of disordered molecular phases. Dielectric and absorption spectroscopy techniques reveal that various H-bonded cluster configurations can be formed therein, such as trimers, tetramers, both linear and cyclic [4].

Physicochemical properties of glass-forming materials that differ with respect to various functional group substituents, will be compared. Replacing a hydrogen atom with, for example, fluorine or the CF_3 group in benzene ring, influences not only the phase transition temperatures, but also the very polymorphism [5]. This happens because steric features of molecular conformations, within various homologous families/series as well as among their isomers, have fundamental impact on the properties of thermodynamic phases of the respective compounds, with consequences to their possible industrial/pharmaceutical applications. As far as the latter is concerned, general studies of the nature of glass of disordered phases and recrystallization phenomena are particularly important due to similarity in chemical structure and molecular geometry between many pharmaceuticals and alcohols or liquid crystals.

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Monday 28 VIII

Molecular ordering and relaxation dynamics in liquid crystal based nanocomposites

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We report optical polarimetry (linear and circular birefringence) and dielectric studies of nanocomposites representing liquid crystal (LC) materials of different types embedded into tabular nanochannels of silica and/or alumina porous membranes. We aim to explore the molecular ordering, structural transformations and relaxation dynamics of both chiral and nonchiral LCs in a cylindrical nanoconfined geometry. Whereas these materials in their bulk state are characterized by first order transitions from the isotropic to nematic, smectic or chiral nematic (cholesteric) phase, the thermotropic behavior of the confined LCs, explored in a channel radii roughly less than 20 nm, deviates substantially from bulk behavior. There is no isotropic state. The orientational order inside the nanochannels results in an excess birefringence, which is proportional to the nematic order parameter. It evolves continuously on cooling with a precursor behavior, typical of a paranematic state at high temperatures. We demonstrate that the strength of the nematic ordering fields σ, which is inverse to the pore radius R ($\sigma \sim 1/R$), is characterized by a critical threshold ($\sigma_c = ½$) that separates discontinuous from continuous paranematic-to-nematic behavior, i.e. in agreement with the predictions of the phenomenological approach [1].

In contrast to conventional nonchiral nematics, the thermotropic behavior of cholesteric or ferroelectric LCs (SmC*-phase) is characterized by large circular birefringence (optical activity) in their confined state indicating thus a formation of long-periodic helical structures along the nanochannel that accompany the orientational order detectable, particularly, in linear birefringence measurements. The anchoring type at the liquid-solid (pore wall) interface appears to be crucial in the formation of confined helical structures. For normal anchoring a radial-escape structure evolves upon cooling. For tangential anchoring, a large optical activity indicates a continuous paranematic-to-cholesteric transition compatible with the formation of double-twist helices.

Dielectric measurements, on the other hand, provide knowledge about the dynamical properties of the confined LCs, particularly, on their relaxational dynamics which turns out to be quite inhomogeneous. It is slow at the pore wall interface and fast in the center of the pore filling. The strengths of the slow and fast relaxations provide thus local information on the orientational order. The thermotropic behaviour in the core region is found to be bulk-like, i.e. it is characterized by an abrupt change of the nematic order at the paranematic-to–nematic transition. By contrast, the interface ordering exhibits at this transition a continuous evolution. Accordingly, the phase behaviour of LC based nanocomposites can be quantitatively described by a linear superposition of these distinct nematic order contributions.

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Monday 28 VIII

Structure formation in two-dimensional systems of bent-core particles

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In the presentation, we show the role of excluded-volume interactions for the stabilization of liquid crystalline structures in a two-dimensional systems of hard bent-core particles. In the first part, we present results of studies involving particles composed of two arms [1]. We investigate how their details (the apex angle, the type of the arm edges and the thickness) affect the stability of different structures. Using Onsager's Density Functional Theory and constant-pressure Monte Carlo simulations we show that the observed phases are dominated by the antiferroelectric smectic. For very thick particles, however, two different phases are expected: smectic A and ferroelectric smectic. The most interesting is the identification of the nematic splay-bend phase, which is more stable than smectics for particles with thin arms and large opening angles. In the second part of the presentation, we discuss the case of three-arm particles with conformational degrees of freedom, which can dynamically adopt two states: a chiral (*trans*-) and an achiral (*cis*-) one. Our model [2] is a generalization of studies in which both states were considered separately [3]. Using both computer simulations and theoretical approach we show that the system composed of such particles exhibits a rich spectrum of nematic and smectic phases. As in the previous case, we identified stable nematic splay-bend phase. Analysis of the average fractions of conformers in all phases show that in the isotropic phase all fractions are equally probable, the smectic phases are dominated by chiral particles and the splay-bend phase is dominated by achiral ones.

Acknowledgments

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ABSTRACTS

Tuesday 29 VIII

Tuesday 29 VIII – Invited Lecture

Nonlinear spin-lattice coupling in $EuTiO_3$: novel two-dimensional magneto-optical device for light modulation

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$EuTiO_3$ is antiferromagnetic at low temperature, namely below T_N=5.7K. In the high temperature paramagnetic phase the strongly nonlinear coupling between the lattice and the nomnially silent Eu $4f^7$ spins induces magnetic correlations which become apparent in muon spin rotation experiments [1, 2] and more recently in birefringence measurments [3, 4] in an external magnetic field. It is shown here, that high quality films of insulating $EuTiO_3$ deposited on a thin $SrTiO_3$ substrate are versatile tools for light modulation. The operating temperature is close to room temperature due to the cubic tetragonal phase transition [5] and admits multiple device engineering. By using small magnetic fields birefringence of the samples can be switched off and on. Similarly, rotation of the sample in the field can modify its birefringence Δn. In addition, Δn can be increased by a factor of 4 in very modest fields with simultaneously enhancing the operating temperature by almost 100K. The results can be understood in terms of paramagnon phonon interaction where spin activity is achieved via the local spin-phonon double-well potential.

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Nonlinear optical diagnostic of the condensed matter

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One of the condensed matter diagnostic methods is the measurement of nonlinear optical parameters, especially the second harmonic (SHG) and higher harmonics of laser light. The basic schematic of the test station for study of the intensity of harmonic generation of the light is shown in Fig. 1. The harmonic generation of the light was investigated in the reflected light of the primary laser. For second and third harmonic measurements, 20 ns pulsed Nd:YAG laser was used which generating a wavelength of 1064nm with energy up to 400mJ and a repetition rate of 20Hz. The SHG measurement method requires non-centrosymmetric electron structure of the tested materials and nonlinear effects are described by the third order polar tensors [1]. Of course, there is a possibility to disturbing the symmetry of the electron structure by, for example, doping or photoinduction, which results in increased optical susceptibility [2,3]. The paper presents SHG measurements for the powders, single crystals and low-dimensional materials in the form of thin layers. The construction of the material determines the preparation of test specimens and the measurement procedure.

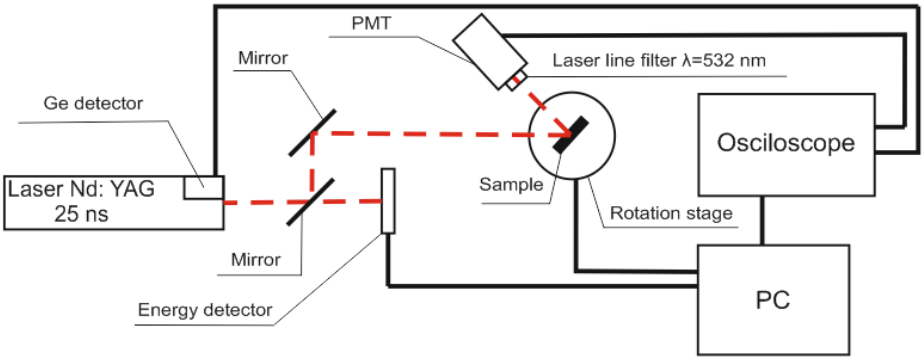

Fig. 1. Measurement scheme for the second and third harmonic generations of the light

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Tuesday 29 VIII

Polymers for ternary organic solar cells

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Constant increase in electricity demand, due to technological progress and rapid population growth, have contributed to growing demand for energy. Because of importance of protecting the natural environment, renewable energy sources, including photovoltaic cells, have become popular. Three generations of photovoltaic cells are developed (silicon, so-called semiconductor thin-layer cells and third generation: dye and polymer cells). Despite the fact that still the first generation silicon cells are still commercially common, more and more popular became organic photovoltaic's (OPV) as one of the most promising technologies for the low cost energy production[1], [2].

One of the research trends is the ternary mixture used as active layers in bulk heterojunction solar cells [3]. Typical active layer is produced by blending conjugated polymers (donor) with high electron affinity molecules (acceptor) like fullerene derivatives[4]. The motivation for creating ternary systems is above all relatively low narrow spectral overlap of organic polymer absorption.

Results for active cell with two component (with fullerene and non-fuleren acceptor) and ternary systems based on pyrazolequinoline derivatives [5] will be presented. Experimental results on ternary systems will be presented as well as a model optimization [6] of such mixtures .

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Photo- and upconversion luminescence in glass-ceramics doped with rare earth elements

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1) To the best of our knowledge, in this work for the first time initial glasses of the potassium-zinc-aluminum-silicate system co-doped with Eu^{3+} and Yb^{3+} were synthesized, transparent glass-ceramics (GC) containing volume precipitated ZnO nanocrystals were prepared by secondary heat-treatments of these glasses and their structure and spectral luminescent characteristics were studied.

In recent years, there has been increasing interest in the development of rare earth (RE) ions doped ZnO quantum dots. RE doped (GC) containing ZnO nanosized crystals are alternative materials to RE ions doped ZnO quantum dots as oppositely to quantum dots, ZnO nanocrystals are homogeneously distributed within the glass matrix without agglomeration.
The luminescence properties of the glass and glass-ceramics were studied by measuring their excitation and emission spectra at 300, 78, and 4.2 K. Strong red emission of Eu^{3+} ions dominated by the $^5D_0$–$^7F_2$ (612 nm) electric dipole transition was detected. Changes in the luminescence properties of the Eu^{3+}-related excitation and emission bands were observed after heat treatments. The ZnO nanocrystals showed both broad luminescence (400–850 nm) and free-exciton emission near 3.3 eV at room temperature (Fig.1). The upconversion luminescence spectrum of the initial glass was obtained under 976 nm laser excitation.

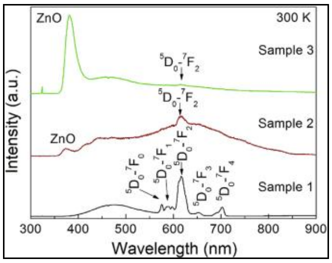

Fig. 1. Luminescence spectra of the glass (the sample 1) and GC (samples 2, 3) recorded at room temperature under excitation of 325 nm laser.

2) Novel transparent oxyfluoride germanosilicate glass-ceramics containing Er:PbF_2 nanocrystals are synthesized on the basis of the SiO_2–GeO_2–PbO–PbF_2 initial glass doped with Er_2O_3 by a secondary heat treatment. The absorption spectrum of the as-cast glass and GC is studied in details. GC is characterized by an intense yellow-green emission, which is enhanced 150 times with respect to the as-cast glass. The redistribution of intensity between the green and red emissions with the heat treatment is explained from the point of view of the lifetime measurements. The UCL in the blue-violet region is also detected. The mechanisms of the UCL for 11 lines in the UV, visible, and near-IR are explained.

Tuesday 29 VIII

Structural and vibrational signature of the suppression of cooperative Jahn-Teller distortion in $TbMn_{1-x}Fe_xO_3$

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Perovskites, with general formula ABX_3, are outstanding materials because they exhibit a rich variety of phases, including ferroelectricity, different magnetic orders, multiferroic properties, colossal magnetoresistance and superconductivity, among others. In many cases, the structure of the low symmetry phase has a Pnma symmetry and the static distortions presented in these compounds are described as tilting of the BX_6 octahedra, involving rotations about the $[101]_{pc}$ and $[010]_{pc}$ axes [1]. These rotations are assigned to the two principal order parameters, with symmetries given by the irreducible R4+ and M3+ representations [1]. Another distortion, which occurs for Jahn-Teller active B-cations, is the cooperative Jahn-Teller distortion that has the symmetry of the M2+ irreducible representation [1]. The cooperative Jahn-Teller distortion is a matter of great interest in the study of many perovskites as it has prominent effects on the lattice, electronic and orbital degrees of freedom, which are correlated to magnetic anisotropies underlying rich magnetic and multiferroic phase diagrams.

A linear relation between the rotation angle and the frequency of the Raman modes assigned to the BO_6 rotations about the $[101]_{pc}$ and $[010]_{pc}$ axes was found for $RMnO_3$ and for $RFeO_3$, which does not exhibit Jahn-Teller distortion [2]. However, it is worth to stress that in despite the R4+ and M3+ distortion mode amplitudes versus the octahedra rotation angle follow a unique linear relation, the proposed rational between the frequency of octahedra rotational Raman modes and the actual octahedral rotation angles is not the same for both families. This unique linear contrasts with the different linear relations observed for rotational Raman modes as a function of the octahedra rotation angle for the different systems [2]. So, it is still not completely clear whether the frequency of octahedral rotational modes images the variations of the octahedral rotation angles, when the cooperative Jahn-Teller distortion is present or not.

Our work aims at a detailed examination of the evolution of the structural distortions as a function of the Jahn Teller distortion for a fixed tolerance factor in $TbMn_{1-x}Fe_xO_3$, from $x = 0$ to 1. Here we report a structural and lattice dynamic study of this system using XRD and Raman scattering at room conditions, evidencing its structural and vibrational signature of the cooperative Jahn-Teller effect, in order to unravel its role on the structural distortions of orthorhombic perovskites.

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Phonon spectra of the HgTe-based topological insulators

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The HgTe and its solid solutions with CdTe or ZnTe in some composition range grown in the form of thin layers or nanostructures exhibit new properties such as those shown by topologically insulators or massless fermions layers with the Dirac points [1] which properties could be astonishing from application point of view. The phonon states in such systems are of particular interest because of unexpected singularity in the temperature dependence of the phonon frequency [2].

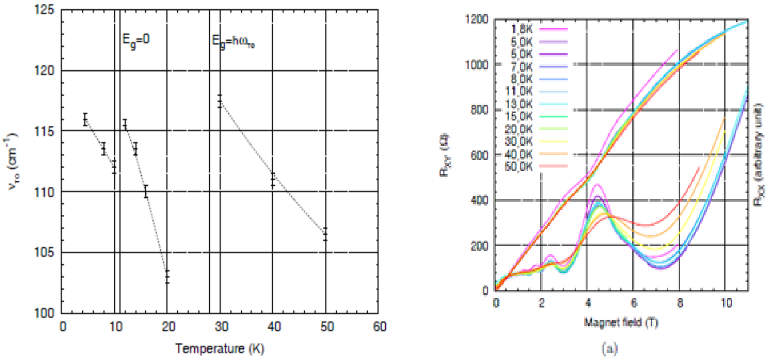

Fig. 1. a) The positions of maxima function Im ε(ω, T) on the frequency scale for sample $Hg_{1-x}Cd_xTe$ (x=0.155); b) magnetoresistance R_{xx} and the Hall resistance R_{xy} in the same temperature region.

This paper presents the experimental results of the magneto-transport (longitudinal magnetoresistance R_{xx} and the Hall resistance R_{xy}, see Fig. 1b) as well as optical refection measurements in the phonon frequency region over a wide interval of temperatures (from 0.4 to 50 K where the Dirac point should occur, see Fig. 1a) for bulk sample of $Hg_{1-x}Cd_xTe$ (x = 0.155) grown by MBE. An amazing temperature stability of the SdH-oscillation period and amplitude is observed in the entire measured temperature interval up to 50 K whereas a discontinuity of temperature dependence of the phonon frequency at the Dirac point (12 K) takes place. It is naturally to assume that the magneto-transport measurement results are mostly attributed to the surface where 2D metallic phase of Topologically Protected States takes place: when the temperature increases above the Dirac point of these states are not disturbed immediately and the electron transport ought to be stable.

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Electrons in a finite two-dimensional system

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Two-dimensional finite system of itinerant electrons interacting via hopping and Hubbard Hamiltonian is considered. The symmetry of the multi-electron states is described by the translation group, symmetric and unitary group. The first mentioned group provides the quasimomentum as an exact quantum number, and two other groups give the total spin of the system. In this way the eigenvalue problem is presented in two symmetry adapted bases, and the operators enabling transformation between them are introduced, with the use of irreducible representations of those three groups.

Role of spin-orbit interaction and strong electron correlations in predicting fundamental properties of advanced nuclear fuel materials for generation-IV reactors

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Uranium carbides have received renewed experimental and theoretical interest for the last few years due to their relevance for nuclear technology. They are recognized as a promising high-temperature fuel materials in the generation-IV reactors [1]. Generally, these carbides exhibit several safety-related advantages and properties superior over those of conventional oxide fuels (like uranium dioxide), which are presently utilized in the nuclear fuel cycle. Despite this certain technological importance, a complexity of phenomena determining fundamental properties of uranium carbides still poses a real challenge for theoretical methods such as state-of-the-art density functional theory. This is mainly because the physics underlying the fundamental properties of these compounds is governed by a competition between the localization and itinerancy of the 5f electrons as well as spin-orbit interactions. Both effects are dominant factors in determining structural, electronic, magnetic, and dynamical properties of compounds from the U-C system. Also, a better understanding of the behavior of 5f electrons remains crucial for description and prediction of the nuclear fuels performance during the in-pile operation as well as for development of modern nuclear fuel materials with desired properties, such as those involving mixed-carbide fuels, like (U, Pu)C.

This contribution presents results obtained for uranium monocarbide within the theoretical approach which considers not only the localized versus itinerant nature of the f-electrons, but also the role of spin-orbit coupling effects [2]. It conclusively demonstrates that the treatment of strong electron and spin-orbit interactions on equal footing remains crucial for proper characterization of such fundamental properties as electronic, mechanical and phonon properties of uranium monocarbide. Results of our theoretical investigations closely correlate with the x-ray photoemission (XPS) and bremsstrahlung isochromat (BIS) spectroscopies [3] as well as the inelastic neutron scattering (INS) experiments [4,5]. The current approach allows to remove the existing inconsistency between theory and experiment and can be applicable to other actinide materials which are relevant for nuclear technology.

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Tuesday 29 VIII – Invited Lecture

Low-frequency dynamics in Pb-based ferroelectric relaxors

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Pb-based relaxor materials (*e.g.* $PbMg_{1/3}Nb_{2/3}O_3$) despite a considerable, two-fold effort (focused on a comprehensive understanding on one hand and replacement on the other) remain important technologically and carry unsolved physical problems. Low energy dynamics is at the core of the relaxational mechanisms in these materials and hence governs their exceptional dielectric properties. There has been a considerable effort to approach low frequency phonons experimentally *e.g.* by means of neutron [1,2] and hyper-raman [3] scattering. A number of puzzling/unconventional features has been observed including so-called waterfall effect (nearly vertical dispersion of optical phonon branch and its collapse onto the acoustic branch) [1], vertical columns of scattering localized at M-points in the reciprocal space [2], Γ-point Raman-active THz modes forbidden in the cubic symmetry[3].

In this work we make use of a recently developed classical shell model potential [4] and run molecular dynamics simulations over times long enough to access those low-frequency features. Having a fully atomistic model allows us to get an insight into mechanisms behind them as well as to study an impact of chemical ordering (Mg/Nb arrangement). We discuss the results in the context of non-relaxor Pb-based perovskites like $PbTiO_3$ and $PbZrO_3$.

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Soft and central mode dynamics in relaxor ferroelectric $PbMg_{1/3}Nb_{2/3}O_3$: dielectric response compared to hyper-Raman and neutron scattering

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Existing infrared (IR) [1] and new IR, terahertz (THz) and available microwave dielectric data [2] on the classical relaxor ferroelectric $PbMg_{1/3}Nb_{2/3}O_3$ (PMN) in the broad temperature range of 10-900 K are combined and fitted using several phenomenological models including models based on effective medium approximation (EMA) [3]. The soft and central mode data are compared with the recent hyper-Raman scattering (HRS) [4] and inelastic neutron scattering (INS) data [5,6]. Despite of macroscopically cubic structure of PMN for which only 3 F_{1u} polar modes are IR active, more modes were resolved in the IR spectra due to locally reduced symmetry. The IR and THz spectra show qualitative agreement with HRS concerning the number of observed modes below ~100 cm^{-1} (2 and 3 above and below room temperature, respectively) and their temperature behaviour, but reveal some quantitative differences. Particularly, the low-temperature data show somewhat higher frequency of the A_1-component of the soft mode [3] and of the extra mode, interpreted as the F_{2g} Raman and HRS active mode [4] activated due to locally doubled unit cell. Our IR-THz data were successfully interpreted within the EMA approach based on the presence of anisotropic polar nano-regions [3]. Good fits using EMA modelling require 4 (A_1+E) modes above 300 K as in Ref. [3] and another weak (A_1+E) doublet at 70-80 cm^{-1} at low temperatures, which could originate from the F_{2g} mode. It appears that an additional relaxational central mode emerges from the low-frequency E-component of the soft mode below ~400 K and splits on cooling into two components, of which the lower-frequency one slows down and broadens towards the freezing temperature, whereas the higher-frequency one broadens, but remains at high frequencies above ~10^7 Hz down to 100 K. Maximum soft-mode contribution to the low-frequency permittivity occurs near 400 K and amounts to ~2,000, whereas the low-frequency permittivity maximum of ~25,000 near 235 K is predominantly due to the contribution of the lowest-frequency relaxation.

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Electromagnons in multiferroics with Y- and Z-type hexaferrite structures

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The microscopic origin of the ***static magneto-electric coupling***, i.e. the change of magnetization with electric field or of polarization with magnetic field, is already well understood. Depending on the specific magnetic structure of the investigated materials, the exchange striction ($\propto \mathbf{S}_i \cdot \mathbf{S}_j$), the inverse Dzyaloshinskii-Moriya (D-M) interaction ($\propto \mathbf{S}_i \times \mathbf{S}_j$) or the spin-dependent covalency between the metal *d* state and ligand *p* state may play the key role. In contrast, due to the ***dynamic magnetoelectric coupling***, magnons can be excited in THz spectra by the electric component of the electromagnetic radiation; therefore, these excitations are called ***electromagnons*** and contribute to permittivity.

Interestingly, different coupling mechanisms can be responsible for the static and dynamic magnetoelectric couplings in the same material. For example, in $TbMnO_3$, the static polarization is induced along the crystallographic ***c*** axis by the inverse DM interaction due to a noncollinear spiral spin structure. Nevertheless, due to exchange striction, two broad electromagnons activate in the E||a polarized THz dielectric spectra. [1]

We investigated experimentally the *Y*-type hexaferrite $BaSrZnCoFe_{11}AlO_{22}$ and the *Z*-type hexaferrite $(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$. Near room temperature, a small applied magnetic field ~ 0.01 Tesla induces a transverse conical ferrimagnetic structure where the inverse DM interaction is responsible for the appearance of a static ferroelectric polarization in the hexagonal plane. Electromagnons activate due to exchange striction in the E||c polarized THz spectra already without external magnetic field although magnetic structures in the Y- and Z-type hexaferrites are different. [2] Above 2-4 Tesla, the electromagnons and the static polarization disappear, because the magnetic structure transforms to a collinear one.

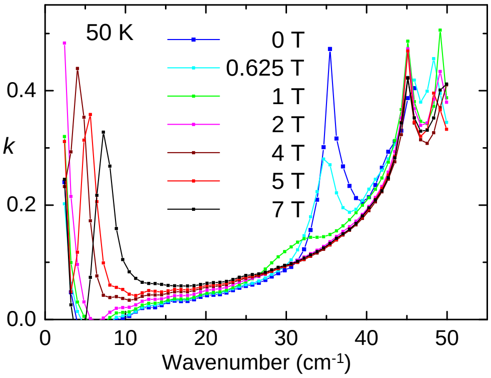

Fig. 1. Magnetic field dependence of the extinction coefficient in Y-type hexaferrite $(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$. The electromagnon near 35 cm^{-1} (~1 THz) gradually broadens with *H* and disappears for $\mu_0 H > 2$ T. The ferromagnetic resonance seen below 10 cm^{-1} (~0.3 THz) shifts linearly with *H*, while the phonon near 45 cm^{-1} is stable in *H* (after Ref. 2).

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Relaxations in uniaxial relaxor ferroelectric SBN

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Relaxor ferroelectrics are known for their extraordinary dielectric and electromechanical properties, widely used in industrial applications ranging from micro-capacitors to transducers and actuators. At the same time the fundamental understanding of their behaviour at a microscopic level, involving disorder effects and nanoscale structural correlations, remains one of the challenges of contemporary solid state physics.

We have studied a single crystal of the uniaxial relaxor SBN61 ($Sr_{0.61}Ba_{0.39}Nb_2O_6$) by neutron backscattering in the sub-GHz range in order to explore its dynamic behaviour in the vicinity of the glass-like ferroelectric phase transition. We have found that one of the two known transverse diffuse scattering contributions [1] in the (001) Brillouin zone is quasielastic. The characteristic frequency of the polar fluctuations and its temperature dependence corresponds to a Cole–Cole relaxation, specific for relaxors, which is known to produce a major contribution to the high dielectric permittivity of SBN61 [2]. Our results provide direct evidence that the ‘critical’ relaxation with its Vogel–Fulcher-type frequency dependence of dielectric permittivity is associated with dynamic nanoscale polarization fluctuations. The results will be compared with those from the cubic relaxor PMN-xPT ($Pb(Mg_{1/3}Nb_{2/3})O_3$ – x% $PbTiO_3$) system.

Acknowledgements: The results presented were obtained in a tight collaboration with coauthors of Ref. 3, i.e. J. Dec, B. Frick J. Combet and M. Appel.

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Switchable perovskite-like crystals with the organic guest

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A family of cyano-bridged coordination polymers (CPs), which undergo transition between the high and low dielectric state upon a thermal stimulus, are promising materials with the potential application in electrical and electronics devices [1, 2]. The carefully designed cage compounds with organic guest molecules as cations, may give materials, where the solid-to-solid phase transitions of different nature, like the order-disorder or displacive one, can be observed. However, it should be noted that the guests should have relatively small dimensions, a spherical form and be endowed with a dipole moment in order to observe the dynamical effects. Moreover the switchable guest cations into the well-matched anionic host framework should possess a relatively large freedom for rotation, i.e. they should have the possibility to jump between at least two energetically equivalent positions. The reorientation of the polar guest may result in the switch of the related physical properties, for example: non-linear optics, changes in electric and magnetic susceptibility and electric polarization. The cyano-bridged coordination polymers (CPs) are classified as an elaposolite family, the typical structural feature of which is a presence of the octahedral groups, as shown in Scheme 1. Some examples will be shown and discussed [3].

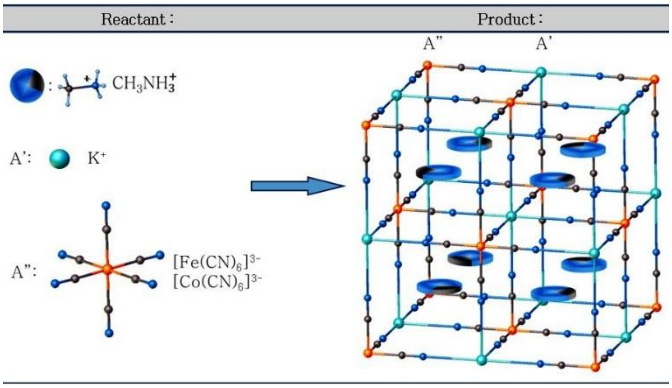

Fig. 1. Typical structure of the cyano-bridged coordination polymers.

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Dynamic properties of Co doped barium titanate

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Cobalt doping into ferroelectric barium titanate may be interesting method for obtaining new materials with both ferroelectric and magnetic properties. Ceramics (1-x) $Ba_{0.95}Pb_{0.05}TiO_3$ + xCo_2O_3 and (1-x) $BaTiO_3$ + xCo_2O_3 were prepared by hot sintering method in ambient air. For the obtained samples many physical properties in complementary manner were studied [1-4]. The results from FTIR should be emphasized because they are compatible with the results of DSC, DMA, magnetic and dielectric measurements. The changes in *e.g.* five Lorentz-shape lines in the 450-950 cm^{-1} frequency region show changes which agree with the phase transitions observed in DSC or dielectric measurements [3]. A peak at about 490 cm^{-1} at the lowest temperatures arises from rhombohedral structure of crystalline phase. Changes of the structure and the symmetry of phases determine the changes of dynamics and, at the same time, different spectra obtained for different phases. The changes of the structure imply changes in the neighbourhood of the oxygen atoms that is marked as a peak on the spectra. Shift of O^{2-} ions, causing a deformation of the structure in the very low temperatures, corresponds to occurring the clear band at about 490 cm^{-1}.

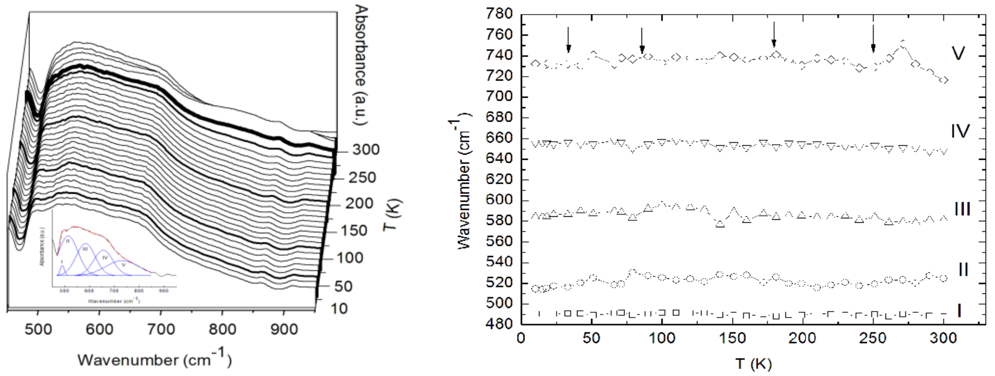

Fig. 1. Left: Experimental FT-IR spectrum of 0.98 $Ba_{0.95}Pb_{0.05}TiO_3$ + 0.02Co_2O_3 recorded in the range from 10 K to 300K. Inset: broad vibrational band at 10 K is fitted with five Lorentz lines in the 450-950 cm^{-1} wavenumber region [2]. Right: Temperature changes of positions of Lorentz function fitted to the broad band in the 450-950 cm^{-1} region [2].

The wider results of the FTIR measurements for two gropus of barium titanate ceramic doped by cobalt oxide with and without small lead amounts will be presented.

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Tuesday 29 VIII

Spin waves in low dimensional inhomogeneous nanostructures

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There is a continuous interest in a size reduction of the magnetic data storage devices. The most promising route to the miniaturization is offered by modern spintronics, also based on molecular magnetic materials, that allows one to control the architecture of individual spin arrangements to an unprecedented precision. In the poster we will present elementary excitations in selected linear and branched chains of spins consisting of segments differing in strength of magnetic coupling. Different kinds of anisotropy will be also considered. The method of calculations originates from the dynamical matrix technique [1]. The surface and interface response function (Green function) theory [2] will be used to treat the junctions of different segments. The surface and/or interface excitations (magnons) correspond to poles of the appropriate Green functions. For some parameters the excitations appear on the background of the bands of bulk waves, whereas in other cases they transform into finite-lived interface resonances. We also calculate reflection and transmission coefficients for the magnons at the junctions.

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Relativistic response and coupled spin-charge plasmon at the Tl/Si(111) surface

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A key simplifying idea or approximation of contemporary many-body physics has been the concept of the collective mode. Among others, the so-called plasmon and magnon states have been historically considered separately as the collective modes associated with the real-space oscillations of charge and spin densities, respectively. However, relativity is known to introduce a peculiar interplay between the electron charge and spin, and it has been proven to produce well defined spin-textures even in nominally non-magnetic materials [1].

In this short communication I will present a comprehensive ab initio analysis of the spin-charge correlations at the Tl/Si(111) surface, where the spin-orbit interaction is so strong that a detailed treatment of the non-collinear electron spin appears decisive for the correct description of the response properties. The relativistic limit enforces a unified treatment of the spin and charge densities as a four-vector, and the response function acquires then a 4×4 tensor structure. Our all-electron implementation allows to resolve the real space structure of the possible collective modes, and demonstrates the emergence of a novel plasmon excitation combining transverse-spin and ordinary charge oscillations of a similar order of magnitude, whose spin character is strongly enhanced as we approach the q→0 momentum limit.

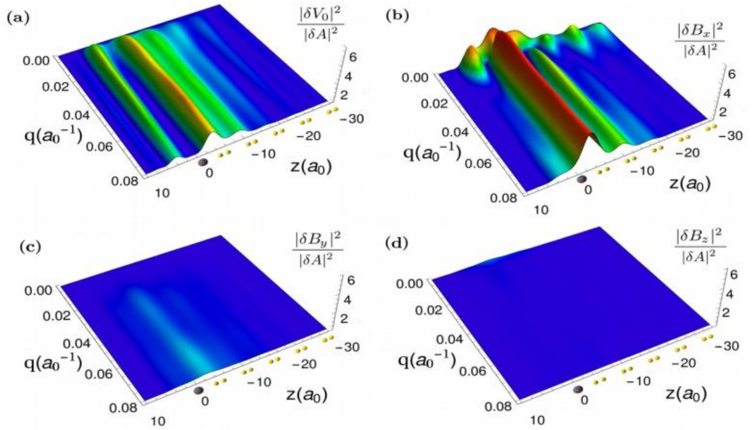

Fig. 1. Real-space structure and momentum (q) dependence of the coupled spin-charge plasmon. The normalized four components of the self-sustained oscillation are shown with respect to the *z* coordinate, the direction perpendicular to the surface. Negative values of *z* correspond to penetration into the bulk, and orientative positions of the first thallium and silicon atomic layers are represented by big gray and small yellow spheres, respectively.

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Dynamics of arteries – effects of occlusions and embolus

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The mechanics of the blood transport in arterial vessels (haemodynamic) involves viscoelasticity of the vessel walls and the rheological properties of blood. The resulting form of the transport shows a wave-like character known from the pulse waves. In what follows the mechanical waveguides are modelled with the use of electric transmission lines.

Arterial embolism (thrombosis), is the most common cause of ischemic strokes [1-3]. After being detached in heart, the particle of the embolus usually travels through the arterial system until it encounters a small enough diameter of the vessel. The resulting blockage of the vessel entails further symptoms related with hypoxia (malnutrition) of the corresponding cells.

Despite the importance of embolism, little is known about the hemodynamic factors that govern the path emboli tend to follow. To reproduce the path of the thrombus, a one-dimensional model of flow and pulse wave propagation was used [4,5]. Our model of the embolic transport is based on Newton’s second law, but in a more specific format termed the Basset-Boussinesq-Oseen equation:

$$m_p\left(\frac{dU_p}{dt}\right)=\frac{1}{2}C_D\rho_F A_P|U_S|U_S+\frac{1}{6}\pi\phi_P^3(\rho_P-\rho_F)g+\frac{1}{6}\pi\phi_P^3\nabla P$$

where m_p is the mass of the particle, ϕ_P and ρ_P are diameter and density of the particle, respectively, dU_p/dt is the particle acceleration, U_p and U_S are velocities of the thrombus and slip velocity between the solid particle and the flowing blood. This equation comes from the fluid mechanics and allows one to describe the influence of blood (fluids flowing in vessels at the average velocity) on the propagation of the thrombus particle [6]. The probability of the occurrence of vessel blockage has been estimated with the use of Monte Carlo method. The calculation takes into account the size and the density of the embolus particle and has been repeated 100,000 times. For the vessels most exposed for embolism, a simulation using a new embolic transport model was performed.

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Weber-Fechner law in short time acoustic pulses

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The Weber-Fechner Law states that the just perceptible difference of two stimuli is proportional to the intensity of the stimuli themselves. (Of course the difference is small as compared to the stimuli). This implies a logarithmic dependence of the sensation on the stimulus intensity [1,2]. In our case, it corresponds to the just perceptible difference in the duration time being proportional to the duration of the pulse. Gaussian pulses may be distinguished by the sensation of the pitch or the timbre [3]. In principle it is not possible to determine simultaneously the pitch and the duration time because of the limitations imposed by uncertainty principle, (Heisenberg [4] as used in quantum mechanics, or Gabor [5] in signal processing) . It is surprising that, despite physical restrictions, humans associate some effective pitch to millisecond pulses up to about 20 ms. The effective pitch has been found to increase with decreasing duration time of the pulse [6]. Musicians and nonmusicians groups have been examined. The behavioural test was held in controlled conditions, where every person used the same software, and used the same audio tools parameters. The participants marked the just noticeable difference in the pitch and the timbre. Statistical analyses of the results will be presented in the communication.

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Tuesday 29 VIII

Raman scattering investigations of phase transitions in the nanocrystals of $PbZrO_3$-$BiFeO_3$ system

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Recently, the origin of antiferroelectricity is widely discussed in literature. Basing on the lattice dynamics in $PbZrO_3$ a phenomenological model with competing interactions between AFE and FE modes was proposed by Tagantsev [1]. It is well know that competing interactions can be strengthened by doping or pressure. Consequently some chemical modifications by different cation replacement can strengthen either FE mode (i.e. Ti4+) or AFE mode (i.e. Sn4+) . Form the available literature it is known that doping of $PbZrO_3$ with $BiFeO_3$ less than 20% does not alter the parent orthorhombic structure of PbZrO3 [2]. $PbZrO_3$ is as classical antiferroelectric with *Pbam* orhorhombic space group [1] whereas $BiFeO_3$ is known as multiferroic possessing rohombohedral *R3m* structure [3]. Such a system system has received some interest in the past [2] primarily due to investigation of the Mössbauer effect which were aimed to solve the problem of the soft mode existence in antiferroelectric crystal [4].

Here we reinvestigate the phase transitions sequence of $PbZrO_3$ substituted with small amount (4%) of $BiFeO_3$ by means of, micro-Raman scattering, dielectric and differential scanning calorimetry (DSC) measurements. Our measurements confirmed that this solid solution undergo two phase transitions within the approximate temperature range 450-500K and about 600K, in agreement with previous findings [2]. Both phase transitions are undoubtedly of first-order character. On the basis of Raman spectroscopy, the symmetry of lower temperature phase was found to be the same as in pure $PbZrO_3$, whereas the intermediate phase of PZO-4$BiFeO_3$ is similar to the antiferroelectric intermediate phase of $Pb(Zr_{1-x}Sn_x)O_3$ solid solution [5]. In next step we will try to explain the mechanisms of the phase transitions existing in the compound with special emphasis for searching of the potential soft mode (or soft modes).

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Ferroelastic domain boundary movement in $PbZrO_3$

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Single crystals of $PbZrO_3$ have been studied by Dynamic Mechanical Analysis measurements in the low frequency range f=0.02 - 50 Hz. Our measurements revealed that the complex Young's modulus shows a different behaviour depending on the direction of the applied dynamic force. In pseudocubic $[100]_c$-direction we found intrinsic elastic behaviour as expected from Landau theory: At the antiferroelectric transition $T_c \sim 510$ K a downwards cusp anomaly in Y_0 accompanied by a peak in Y_{00} points to a quadratic/linear order parameter/strain coupling in the Landau free energy. Both anomalies are increasing with decreasing frequency showing that the measurements are performed in the limit $\omega_{th} > 1$. The low frequency elastic response in $[110]_c$-direction is different. Below T_c we find in addition to the intrinsic anomaly a strong contribution from ferroelastic domains, which leads to an additional softening in Y_0. With decreasing temperatures this superelastic softening gradually disappears, due to the increasing pinning of DW's to defects resulting in DW freezing. Besides, for forces along $[110]_c$ we found a pronounced precursor hardening, starting at about 60 K above T_c. Since this anomaly is of dynamic nature, starting at the same temperature as the observed birefringence and piezoelectric anomalies [1], we conclude that it originates from slow dynamic polar clusters which freeze at $T \sim 550K > T_c$.

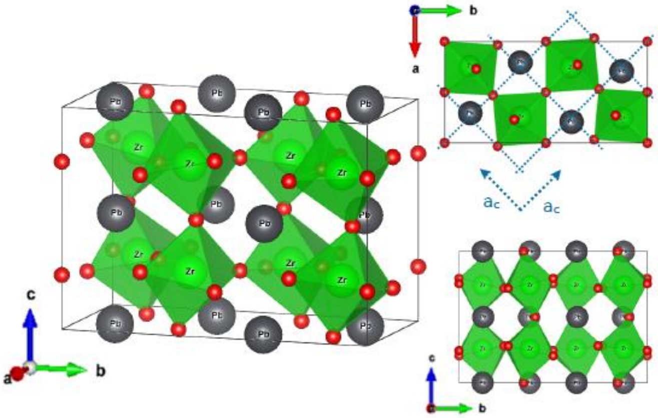

Fig. 1. Crystal structure of $PbZrO_3$ in orthorhombic Pbam phase. The pseudocubic unit cell is indicated by blue dotted lines.

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Theoretical inquiry into the signatures of coherent wavepacket motion in singlet exciton fission

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The singlet fission is the process of radiationless conversion of a singlet excited state into two triplet states entangled into the overall spin singlet. It occurs in a wide range of organic chromophores in which the energy of the excited singlet happens to be approximately equal to the doubled triplet energy [1]. The process is extensively investigated because it potentially enables an increase (even twofold) of the number of free charge carriers generated in photovoltaic cells. Despite the numerous studies, there is still no consensus on the mechanism of the singlet exciton fission whatsoever.

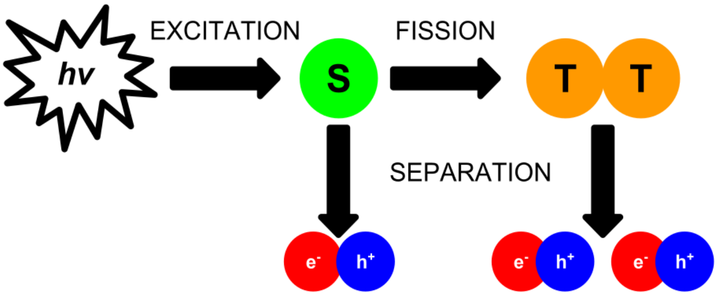

Fig. 1. Scheme of the singlet fission process as a way of doubling the number of charge carriers

In pentacene and TIPS-pentacene films, singlet fission occurs extremely fast (~80 fs timescale). Such ultrafast dynamics was observed by Musser *et al.*, using femtosecond transient absorption measurements which revealed that in the fission process the coherence of the initially excited singlet wavepacket is passed on to the coupled-triplet manifold [2].

We attempted to rationalize why certain normal modes contribute to the measured signatures of vibrational coherence, while others remain in that sense inactive. In order to do that, we performed quantum-chemical calculations of pentacene vibrations in the ground, excited singlet and triplet states. We also constructed a model of the vibrational coherence signatures, based on time-dependent perturbation theory in the wavefunction formulation. When the experimental parameters (pump pulse duration and energy) and the calculated Franck-Condon coefficients were inserted into the model, they yielded semiquantitative indices of vibrational coherence for all totally symmetric normal modes. The results, with minor exceptions, happen to agree with the experimental results mentioned above.

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Tuesday 29 VIII

Relaxation processes occurs in (1-x) 70/30 PZT - (x) $BiMn_2O_5$ ceramics

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The (1-x)$PbZr_{0.70}Ti_{0.30}O_3$ - (x)$BiMn_2O_5$ ceramic series was studied for x = 2, 5, 11, 15, 22 %. We determined electrical properties of PZT material influenced by non–polar BM addition. The electric impedance was measured for frequencies f = 0.1 Hz – 1 MHz in the 100 – 600 K range. Value of real part of permittivity ε′ monotonically increased for ceramics, which contained bismuth manganite. One relaxation process was detected for non-doped PZT sample. The estimated relaxation times varied in 10^{-6} – 10^{0} s range. This process in the samples was assigned to the electrical conductivity dispersion and to participation small polarons in electric transport The addition of bismuth manganite induced the second relaxation process in other samples. The determined relaxation times depended on the chemical composition of the samples. The induced relaxation exhibited relaxation times in 10^{-7} – 10^{-1} s range. The occurrence this relaxation process is attributed to the BM doped to the PZT ceramics. Activation energy was 0.81 eV for pure PZT and changed from 0.36 – 0.89 eV for doped samples. Temperatures of structural phase transitions were determined for the 0.98PZT–0.02BM and the 0.945PZT–0.055BM ceramics.

Peculiar thermal transport of 1-fluoroadamantane

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The polymorphic nature of a plastic crystal of 1-fluoroadamantane has been studied by the means of thermal conductivity, heat capacity and differential scanning calorimetry. The original results of temperature dependency of thermal transport properties have revealed a curious phenomenon while changing the cooling procedure. Namely, on single cooling of the orientationally disordered phase from room temperature down to liquid helium temperatures, 1-fluoroadamantane exhibit features characteristic for crystalline materials. However, going back above the phase transition point (227K) changes the temperature dependency of thermal conductivity coefficient by introducing the new type of disorder. Crossing that temperature point has caused the irreversible transition towards the low temperature disordered phase and simultaneously variating the observed features into an amorphous like. The other unique result is the anomaly around 185K, which was reported in all the investigated properties. Authors recognize the observed change as an evidence of a possible glass transition. The presented results are first experimental proofs of particular low temperature polymorphic states of 1-fluoroadamantane (ordered- and disordered- phases). The detailed analysis of our investigation will be carried out based on thermal transport mechanisms.

Tuesday 29 VIII

Impedance spectra of the $Na_{0.5}Bi_{0.5}TiO_3$ single crystals and ceramics

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The sodium bismuth titanate $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) is one of the most promising lead-free material for piezoelectric devices and electro- mechanical transducers. Recently it was found that electrical properties of NBT single crystal were dependent on atmosphere and temperature of thermal treating [1]. The results obtained in [1] indicate the presence of associated dipole complexes and mobile charged defects, which include oxygen vacancies in NBT crystals.

In the abstract we report the effect of heat treating in air on conduction mechanisms of NBT crystals and ceramics. Measurements were carried out in the temperature interval 600-900 K and in the frequency range $5\text{-}5\cdot10^5$ Hz by Tesla BM-507 impedance meter. Experimental data were obtained in the regime of thermal stabilization.

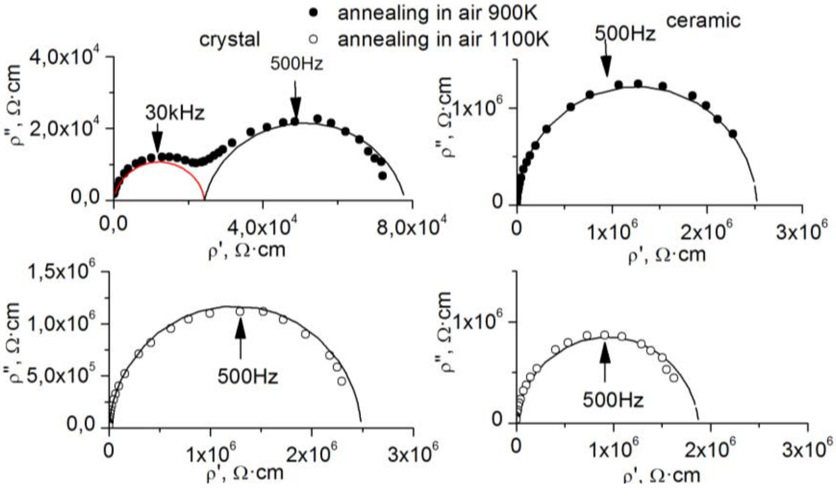

Fig. 1. Impedance spectra of NBT for single crystals and ceramics, T = 820 K

It is proposed that high-frequency arc on the hodographs of NBT crystals is associated with conductivity in the bulk of the sample. The low-frequency arc reflects the charge transfer in the near electrode regions. However, only the low-frequency arc is observed on crystals annealed at 1100 K. The low frequency arc on the hodographs of NBT ceramics may be reflects conduction within intergrain regions. The effect of heat treatment on the conductivity mechanisms of NBT crystals and ceramics is discussed.

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Tuesday 29 VIII

Correlation of the magnetic structure modulation with the magnetoelectric behavior of $TbMn_{0.98}Fe_{0.02}O_3$

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Multiferroic materials have received large attention in the last decades because of the fascinating coupling between magnetism and ferroelectricity, which have promoted the flourishing of different theoretical models to understand their properties. One of the most studied multiferroic materials has been $TbMnO_3$ [1]. At $T_N = 41$ K, $TbMnO_3$ undergoes a magnetic phase transition into an incommensurate antiferromagnetic phase, with a longitudinal spin density wave propagating along the a-axis (Pbnm setting) [1]. Below $T_{lock} = 26$ K, a commensurate cycloidal magnetic order in the bc-plane becomes stable, which allows the emergence of spontaneous electric polarization along the c-axis, according to the Dzyaloshinskii-Moriya mechanism [1]. $TbMnO_3$ also exhibits a ferroelectric polarization flop when a high enough magnetic field is applied along the a- or b-axes [1].

The Mn^{3+} substitution by the non-active Jahn-Teller Fe^{3+} in $TbMnO_3$, even in small concentrations, is an effective route to reach a substantial change of its magnetic properties [2]. Due to the fact that both Mn^{3+} and Fe^{3+} ions have the same radius, a fully solubility is obtained. However, since their magnetic properties are very distinct, the magnetic phase diagram of $TbMn_{1-x}Fe_xO_3$ is strongly dependent on Fe^{3+} content [2]. The most remarkable result is the reduction of the electric polarization as x increases and its total suppression for $x \geq 0.05$. This result has been assigned to the unbalance of the competing magnetic interactions towards the ferromagnetic ones, promoting a weak-ferromagnetic character, which destabilizes the cycloidal spin modulation, necessary for the appearance of the electric polarization [2]. Interestingly, the magnetoelectric effect in $TbMn_{1-x}Fe_xO_3$, $0 \leq x \leq 0.04$ greatly increases, in which the electric polarization becomes much more susceptible to an applied magnetic field with increasing x. Thus, the mechanisms underlying this effect deserve experimental study, namely the magnetic field induced lattice distortions and spin arrangements in order to get a deeper knowledge regarding the spin-lattice coupling.

This work aims at unravelling the effect of Fe^{3+} substitution in the magnetoelectric properties of the $TbMn_{0.98}Fe_{0.02}O_3$, by accurately ascertaining the changes of both crystalline and magnetic modulated structures, along with their commensurable character, through single crystal neutron diffraction studies as a function of both temperature and magnetic field. This will allow to correlate these modulations with the emergent ferroelectric properties and namely explain it becoming more susceptible to an applied magnetic field.

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Tuesday 29 VIII – Invited Lecture

Hydrogen motions in defective graphene: the role of surface defects

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Hydrogenated graphene sheets, produced in macroscopic quantities by the thermal exfoliation of graphene oxide, have structures that show a high degree of disorder and they are therefore poorly characterised. The key interest in this system is as a catalyst for the formation of molecular hydrogen in interstellar clouds. Neutron vibrational spectroscopy, combined with DFT molecular dynamics simulations, provides a fingerprint of the local structure. sp^2 carbon sites, on the edges of and in voids in the graphene sheets, are clearly identified and the level of hydrogenation is ∼50%. At 5 K, the ground state is composed of large clusters of hydrogen and, at temperatures of ∼300 K, a high degree of dispersion of the clusters is observed. The underlying hydrogen dynamics involves the breaking and reforming of covalent bonds which, at such low temperatures, is mediated by incoherent tunnelling of hydrogen. Understanding the mobility of H at a quantum level is one of the essential ingredients for a robust comprehension of the catalytic formation of H_2 by carbon nanostructures [1].

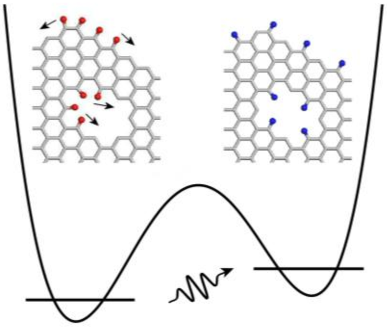

Fig. 1. Schematic representation of the model used in the study to interpret the INS data: phonons from the carbon framework sustain the tunneling of the hydrogen atoms from a compact configuration at base temperature (left model -red) to a dilute configuration at larger temperatures (right model - blue).

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Polymers with different topologies in confined geometries

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Taking into account the well known polymer-magnet analogy developed by de Gennes [1] between the field theoretical φ^4 O(n)-vector model in the limit n-> 0 and the behavior of long-flexible polymer chains with excluded volume interactions in a good solvent the investigation of a dilute solution of long-flexible linear and ring polymer chains in confined geometries like slit of two parallel walls [2,3] or in the solution of mesoscopic colloidal particles of big size with different adsorbing or repelling properties in respect to polymers is discussed [4,5]. We applied the massive field theory approach in fixed space dimensions d=3 for the investigation of the interaction between long flexible polymers with different topologies and mesoscopic colloidal particles of big size and for the calculation of the correspondent depletion interaction potentials and the depletion forces between confining walls. The presented results indicate about the interesting and nontrivial behavior of linear and ring polymer chains in confined geometries and give possibility better to understand the complexity of physical effects arising from confinement and chain topology which plays a significant role in the shaping of individual chromosomes and in the process of their segregation, especially in the case of elongated bacterial cells. The obtained results are in good qualitative agreement with previous theoretical investigations and with the results of Monte Carlo simulations and can find practical application in new types of nano- and micro-electromechanical devises.

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Tuesday 29 VIII

Ellipsometric study of thin films

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Spectroscopic ellipsometry (SE) is a measurement technique that uses polarized light to characterize thin layers, surfaces, and microstructure of materials. This technique allows to specify: optical constants of material (n, k), thickness of thin layers, surface roughness, depth profile of material properties. The advantages of ellipsometry are high precision (accuracy up to 0.01 nm),fast real-time measurements, and wide range of applications. Another important advantage is the fact that during the measurement the sample isn't destroyed. SE also has some disadvantages. One of them is a necessity of fitting the optical model for data analysis which complicates obtaining parameters characterizing the sample.

Optical properties of thin films on soda lime glass substrate were investigated using spectroscopic ellipsometry. Thickness and dispersion relations of optical constants (n, k) were determined. An optical model for coatings on glass is presented and it can be applied for subsequent investigations.

Tuesday 29 VIII

Dynamics of isolated hard nanoparticles stabilized by organic ligands as seen by Mössbauer spectroscopy

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We report on semiconductor nanoparticles, which form systems consisting of isolated hard particles (inorganic cores) embedded in a soft network of stabilizing ligands. Such nanoparticles are interesting by themselves as they provide insight into intermediate level dynamics between atomic and macroscopic scales.

As an example, we have analyzed chalcopyrite-type (Cu-Fe-S_2) ternary nanocrystals stabilized by long aliphatic chain ligands. The main attention has been paid to the behavior of the particles whose average size has varied in a controllable manner from 3 to 20 nm. Dynamics of nanoparticles have been studied by applying Mössbauer spectroscopy.

The fast dynamics can be described by two-level environment. Deeper level (atomic) is found practically the same as for bulk material except Debye temperature. The higher level (particle motion) can be described by the classical harmonic oscillator with the spring constant dramatically softening with increasing temperature. Such behavior leads to fast decrease of the fraction detectable by Mössbauer spectroscopy with increasing temperature. Slow dynamics can be characterized by the thermally driven overdamped harmonic oscillator motions. In addition, the long range-like diffusion of particles is seen. No significant rotation of particles is found within accessible temperature range.

ABSTRACTS

Wednesday 30 VIII

Wednesday 30 VIII – Invited Lecture

Lattice dynamics of rare-earth silicide nanostructures

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The continuous downscaling of CMOS devices imposes severe material and processing challenges and demands a constant search for new self-organized nanostructures. Among the most critical problems are the quality of interconnects, contacts, and the source/drain areas of the transistors. The rare earth silicides became especially attractive for such applications due to their metallic nature and low Schottky barrier heights [1-3]. Deposited on Si(001), depending on the thickness and temperature, some of the lanthanides self-organize in high aspect ratio nanowires, nanoislands and clusters [4].

To address the lattice dynamics modifications of such nano-objects, we have grown epitaxial $EuSi_2$ films and nanoislands [5] and $DySi_2$ films, nanoislands and nanowires [6] and investigated the Eu- and Dy- partial density of phonon states (DOS) by *in situ* nuclear inelastic scattering and first-principles calculations. We found that phonon DOS of the nanoislands [7] and nanowires [8] strikingly deviates from that of the bulk and surface layers and it is to a large extent governed by the atomic confinement at the nanostructure/substrate and nanostructure/nanostructure interfaces. This leads to a remarkable modification of thermodynamic and elastic properties and opens up new avenues for their manipulation.

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The influence of phonons and phasonic flips on the structure factor of quasicrystals

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Quasicrystals are aperiodic structures which undergo two main types of atomic disorder: (*i*) atomic oscillations around equilibrium positions due to thermal vibrations (phonons), and (*ii*) phasonic flips of atoms between equivalent positions (phasons). The latter is a characteristic of quasicrystals [1]. Both phenomena obviously influence the diffraction pattern, which is a reciprocal-space image of the atomic structure, by reducing the diffraction intensities and broadening of the peak profiles. In all modern refinements of quasicrystals based on the higher-dimensional method, likewise of crystals, the correction for all structural disorder (including both phonons and phasons) is made by multiplicative corrective factors, namely the Debye-Waller factor (D-W). It is a standard D-W factor for phonons with exponential form $\exp(-k^2\sigma^2)$, or the so-called perpendicular-space D-W factor in the form of $\exp(-k_\perp^2\sigma_\perp^2)$, where $k_\perp$ is the perpendicular-space component of the reciprocal space scattering vector. We show that the exponential multiplicative factor fails in the context of phasons and it even worsens the refinement result by introducing a characteristic bias in the plot of calculated *vs.* fitted intensities.

In our presentation we show how to include the correction for phonons and, which is even more significant, phasons during the construction of the structure factor formula for quasicrystals. We focus on model systems based on the Fibonacci chain (1D), Penrose (2D) and Ammann tiling (3D case). We apply the statistical method of structural investigation of aperiodic crystals [2,3]. The statistical approach takes a great advantage of the distribution of atomic positions calculated against some reference lattices. The distribution, called average unit cell and denoted as $P(u,v)$, is dense and well defined. It is also highly sensitive to any type of atomic disorder introduced to the structure. Phonons smear a line $v=-\tau^2u$ along [1,1]-direction in (u,v)-space, whereas phasons lead to the fragmentation of marginal distribution $P(u)$. Both effects are easily noticeable. Knowing the fragmentation of $P(u)$ we are able to introduce a phasonic corrective factor at the level of structure factor definition (it is not a multiplicative but an additive factor) with one parameter to fit, which is a number of flips in the structure [4]. In the presentation we will explain the basics of our approach and show how phasonic flips influence the structure factor of model quasicrystals. The interesting results of application of the novel Debye-Waller phasonic correction to model systems will be shown. We also show how strong phasonic disorder leads to random tiling type structure, but with the preserved Bragg-like scaling of peaks, and, eventually, to amorphous system [5].

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Low-temperature phonon anharmonicity in PbTe and (Pb,Cd)Te solid solution

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PbTe is a narrow-gap semiconductor which at the same time is a very efficient thermoelectric material transforming heat into potentially useful electricity. PbTe found several applications e.g., in power generators, infrared detectors, laser diodes or cooling system electronic devices. The origin of its low lattice thermal conductivity has been under extensive debate within the last few years. One explanation of this origin, suggested a strong anharmonic coupling between the LA and TO phonon modes, based on the inelastic neutron scattering (INS) data, determined at room temperature using the time-of-flight technique [1]. Another explanation of the low PbTe lattice thermal conductivity assumed a lowering of lattice local symmetry which explained the observation of a supplementary phonon structure at the Brillouin zone center and in its vicinity [2, 3]. Recently, an important role of the electron-phonon coupling involving electron states near the band edges, leading to the ferroelectric instability in this material was also pointed out [4]. The aim of present work was to investigate the details of the phonon dispersion in PbTe and (Pb,Cd)Te solid solution as a function of temperature below T = 295 K and to analyze the strong TO–phonon anharmonicity, reported previously in the literature. The INS measurements with the use of triple-axis spectrometer were chosen as the experimental technique for that purpose. The high quality PbTe and (Pb,Cd)Te single crystals with the *fcc* structure of the NaCl type, containing 0.6% and 1.9% of CdTe, were prepared by self-selecting vapour growth technique (SSVG) [5]. In order to obtain information on a strong TO-phonon mode anharmonicity both the phonon dispersion and phonon damping along the [001] and [011] directions were determined at temperature range from 3.5 K to 295 K. The softening of TO phonon mode with decreasing temperature was observed at the Γ point of Brillouin zone for both PbTe and (Pb,Cd)Te solid solution. The temperature dependences of other phonon branches are also shown and discussed.

This work was partially supported by the Grant UMO-2014/13/B/ST3/04393 from the National Science Centre (Poland).

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Wednesday 30 VIII

Control of vibrational properties of multilayer phosphorene

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Black phosphorene multilayers attracted enormous attention due to intrisic thickness-dependent band gap and strain tunable electronic structure providing promising device applications. The extreme sensitivity of properties of multi-layer phosphorene to the sample thickness and strain makes determination of the phosphorene flake thicknesses of paramount importance. The relative thickeness and sample orientation can be determined from vibrational analysis of Raman-active low frequency breathing modes existing only in a few-layer phosphorene, which are absent from both monolayer and bulk black phosphorus.

Using standard density functional theory techniques, we study lattice vibrational Raman and infrared modes in strained few-layer phosphorene structure. We find very significant frequency shifts, up to 100 cm-1 in the applied strain range of +-6%, of the non-resonant Raman activities in both high- and low-frequency region and infrared activities in the low-frequency region. The type of applied strain, that is, armchair, zigzag and theirs diagonal combination, selectively affects specific vibrational modes. Combined with high spatial-resolution Raman/infrared scattering experiments, our calculated results can aid understanding of the complicated nature of inhomogeneous strain distributions in few-layer phosphorene or manufacturing of materials with desired electronic properties tunable via strain or layer engineering.

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Not so giant anharmonicity in PbTe

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The problem of anharmonicity in crystals is a long-standing issue in solid state physics. And it is an important one. Nevertheless it does not necessairly warrant sansational headlines in the high-end scientific journals [1]. In this presentation, we show that in the case of PbTe the automatic claim of strong anharmonic effects as a default suspect for any unexplained lattice dynamics phenomenon may not be entairly correct. Furthermore, in light of recent published results [2] and presented calculations the case may be even more complicated than naiively expected.

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Wednesday 30 VIII – Invited Lecture

Phonon anharmonicity

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I shall give an outline of a concurrent approach to anharmonic effects in crystals. The proposed method is free of necessity to expand the interactomic potential over atomic displacements. Using VASP, PHONON and a new anharmonic module I shall show the broadening and shifts, or even the shape of anharmonic peaks as a function of temperature. PThe maps, which can be plotted, can give the impression of anharmonicity distributed over the desired part of Brillouin zones. At higher anharmonicity and in crystals with more atoms in primitive unit cell the anharmonic peaks frequently overlap. Nevertheless a dedicated projection technique can be applied to separate out the peaks consisting of multiple phonon modes.

The procedure is illustrated by showing thermal behaviour of lead, tungsten magnesium silicate, and lead telluride crystals.

Search for superhard materials - importance of the lattice dynamic calculations

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Recent attempts to design new intrinsically superhard materials (H > 40 GPa) concentrated on the introduction of light elements forming strong bonds (B, C, N, and O) into transition metals (T) with high elastic moduli [1]. Here we present the limits of achieved shear and tensile strenghts within 4d,5d T-borides[2], platinium dinitrides[3] and the tungsten carbides with varying stacking sequence[4] using quantum mechanical and lattice dynamics calcualations. The relations between the electronic structure, equilibrium shear moduli, elastic constants, enthalphy of formations and the atomic vibrations are shown. However, to design superhard materials the key factor is the resistance to the plastic flow (plane glide), a situtaion further away from the equilibrium. Recently number of attempts, i.e. addition of boron into diborides, dinitrides of platinium or the variations of atomic planes in carbon-tungsten systems were investigated with the help of the lattice dynamic calculations to demonstrate a possible route to design superhard materials. The origin of the shear strenght's limits and its relation to the electronic structure and their mechanical properties is discussed [2-4].

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Total transmission of elastic waves at solid-solid interface

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When encountering a mismatch of characteristic impedance a bulk acoustic wave transforms into up to three reflected and refracted waves of different polarizations. The effect is known as mode conversion. The lack of the specularly reflected wave is called total mode conversion because then all the outgoing waves propagate at speeds different than that of the incident one, that it's known at the half-space of elastic media [1, 2]. Conversely, if the only outgoing wave reflects in the specular way one speaks of no-conversion. Concurrence of both phenomenons for a particular angle of incident wave results in lack of reflected wave and it is called total transmission. Discovery of materials with negative Poisson's ratio [3] enlarged the range of possible impedance mismatch and of the related phenomena. The conditions for the total mode conversion and no-conversion in reflection and for total transmission will be presented for interfaces between two elastic media. The region of existence of total transmission as well as values of incidence related angles will be presented in relation to the region of existence of Stoneley waves for whole range of Poisson's ratio.

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Wednesday 30 VIII – Invited Lecture

Atomic-scale dynamics in liquid semiconductor alloys

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The physical properties of metallic liquids play an essential role in industrial casting processes, controlling micro-structure evolution and understanding metallic glass formation. The liquid state of alloys is thus a fundamental – yet oft neglected – component of advanced materials processing and design. I will discuss our recent progress in the field of quasi-elastic neutron scattering on liquid semiconductor alloys carried out on the time-of-flight spectrometer TOFTOF at the MLZ in Garching. The unique atomic bonding properties of the semiconductor species can affect the transport properties of the liquid alloy in ways that are useful for materials applications. Results will be discussed with a focus on self-diffusion and structure-dynamics relationships, while also touching on broader themes in the glassy dynamics community such as fragility and dynamic heterogeneity.

Solid or fluid?

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Is it possible that the system in the solid state can be a the same time in the fluid state? Basing on the results from the Onsager theory for a two-dimensional binary system of large and small spherical particles we show the possibility of the phase in which the large particles are regularly arranged in the space while small particles are still in the fluid state. This result depends on the composition as well on the size aspect ratio of large and small particles. Critical values of these parameters for the transition point to the fully solid state has been assessed from the Onsager theory and corrroborated by the study of the dynamical properties from molecluar dynamics simulations.We show also that for certain size aspect ratio and composition hexagonal arrangement of large particles which is typical for a monodisperse system is no longer stable and a square lattice arrangement occurs. The results will be discussed in view of the possibility of the tailored arrangement of colloidal particles on surfaces and their possible application for obtaining thin films with prescribed optical properties.

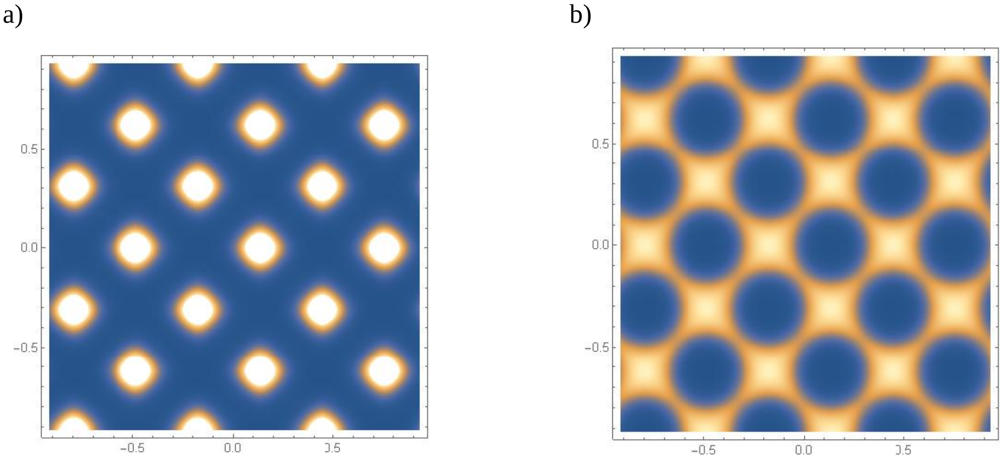

Fig.1. An example of two-dimensional density distribution functions for large particles of the diameter 0.3 a) and small particles of the diameter 0.03 b) in a mixture of 50% large and 50% small particles from the Onsager theory Large particles are well localized on the square lattice whereas small particles encaged in the pores made by the large particles are distributed more uniformly with possibility to move from one cage to another if the large particles are instantly far away to let the small particles to move through the channels between two nieghbouring large spheres.

Porous silica templated nanomaterials for electronics and IT technologies

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The present work is devoted to novel classes of nanomaterials: mesoporous silica thin films containing vertically aligned channels containing functional units or crystalline structures. Such a functionalization makes the materials highly applicative in electronics or IT technologies. We consider three types of silica based materials, containing various functional units in the pores, as shown in Fig. 1.

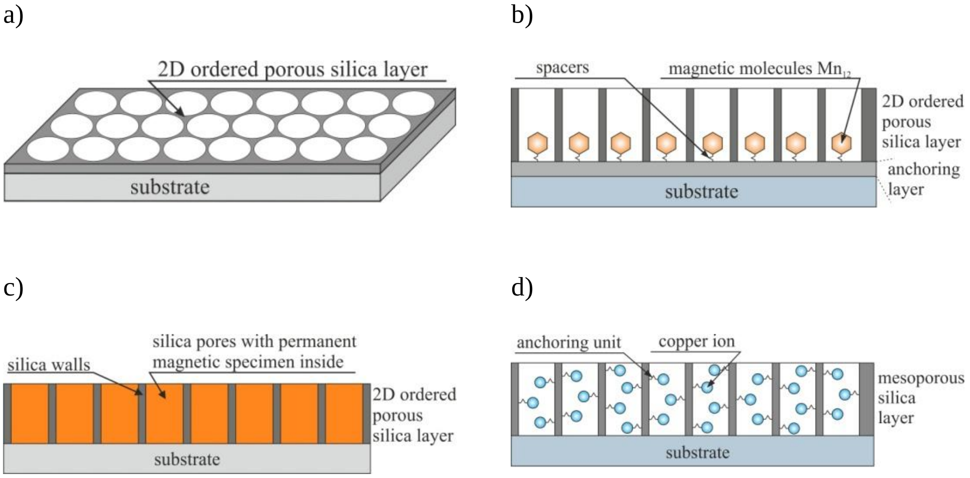

Fig. 1. The structure of silica-templated thin-film materials for electronics and IT technologies: perspective projection (a) and vertical cross section of molecular neurons layout (b), super-dense memory devise (c), material with tuneable non-linear optical response (d).

Porous silica films containing single molecular magnets in pores bottom can play a role of a layout of independent, bistable magnetic units (see Fig. 1b). Such a material can be used as molecular neurons . Similar material containing permanent magnetic specimen inside pores can be use for fabrication of super-dense magnetic memory (see Fig. 1c). Thin silica films with channels arranged perpendicular to the substrate and containing strongly dipolar units (copper phosphonate) have strong non-linear optical (NLO) response (see Fig. 1c). Moreover, NLO susceptibility can be tune by means of functional groups concentration variation. All materials quoted above have strong applicative potential.

ABSTRACTS

Thursday 31 VIII

Thursday 31 VIII – Invited Lecture

Applications of the Raman effect: From femtosecond spectroscopy to waste water analysis

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The Austrian theoretical physicist Adolf Smekal postulated a physical effect in 1923 which predicted that, following the scattering of light from atoms, molecules or crystals, energy would be transferred between the photons and the atoms or molecules being targeted, thereby causing a change in the frequency of the light scattered by the collision. While considering the ramifications of this effect, Smekal assumed that would never be possible to observe this sub-microscopic process as it would take place in just a few femtoseconds.

Nevertheless, just a few years later in 1928, the Indian physicist (and later Nobel laureate) Chandrasekhar Raman was able to demonstrate the frequency shift effect for the first time experimentally. Raman scattering, as the process is known today, forms the basis of one of the most important methods for measuring the vibrational properties of matter with applications from structure determination to waste water analysis. In my talk, I will highlight some of the applications [1], in particular its use for the characterisation of light weight metal hydrides as potential hydrogen storage and battery materials [2]. Interestingly, it has taken almost 100 years to observe in real-time the atomic processes, on which the Raman effect is based. In order to observe the fs short-lived movement in real time, we used a novel experimental technique, combining ultrashort x-ray pulses with an x-ray absorption spectrometer. With this technique we were able to follow the oscillations in lithium ions within the lattice of a lithium boron hydride ($LiBH_4$) crystal excited by a fs-laser pulse [3]. The measured frequency as well as amplitude agree well with the one derived from Raman scattering. The effects in the time domain complete the picture of our understanding of the dynamics of solids usually measured in the frequency domain on one hand; and are a demonstration of the potential of ultrafast X-ray absorption spectroscopy for the study of dynamics in solids on the other.

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Thursday 31 VIII – Invited Lecture

Fractional dynamics in silkworm silk and spider silk

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Structural relaxations in humid silkworm silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional viscoelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history.

An analogous fractional relaxation also gives rise to the subdiffusion observed on picosecond time scales as measured *in situ* using quasielastic neutron scattering (QENS) combined with tensile tests. It describes the mobility of the amorphous polymer chains in silkworm silk and of the adsorbed water on the molecular level in an excellent way. The reduction of the subdiffusive memory effect in stretched fibers compared to native fibers is consistent with the higher order of the polymers in the stretched state [1]. The different morphology leading to the unique mechanical properties of spider silk is reflected in the strain dependence of the fractional dynamics parameters from QENS [2].

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Properties of localized protons in neutron star matter at finite temperatures for realistic nuclear models

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We study properties of the proton component of neutron star matter for a number of realistic nuclear models. Symmetry energy plays a crucial role for composition and some other important properties of dense matter in neutron star. Vanishing of the nuclear symmetry energy implies proton-neutron separation instability in dense nuclear matter [1]. Negative values of the symmetry energy results in disappearance of protons at high densities. There is a possibility of bulk separation of protons and neutrons in neutron star matter.

We also consider the other mechanism of separation which results in localization of individual protons in neutron matter. Protons which form admixture tend to be localized in potential wells corresponding to neutron matter inhomogeneities created by the protons in the neutron medium.

To compare the energy of a normal phase of uniform density and a phase with localized protons we apply the Wigner-Seitz approximation and divide the system into cells, each of them enclosing a single localized proton [2,3]. The neutron density profile is obtained by solving the appropriate variational equation [4]. We performed our calculations at finite temperatures [5]. The localization effect is temperature dependent [6]. Astrophysical consequences of occurring localized protons inside neutron stars are discussed.

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Thursday 31 VIII – Invited Lecture

Gas sensing via chemoresistive effect in nanostructured semiconductors

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The great challenge of low-dimensional nanostructured materials lies in the control of their properties by the morphology and the grain size, which combines bulk and surface effects [1, 2]. One-dimensional (1D) nanostructures are ideal for investigating the dependence of electrical transport, mechanical and optical properties on size and dimensionality [3], i.e., lower turn-on voltage for field emitters, higher efficiency for solar cells, better electrochemical performance for lithium-ion batteries and enhancement of thermoelectric figure of merit. Two-dimensional (2D) nanostructures, i.e., nanosheets, nanoplates, and nanowalls, are suggested to be ideal components for nanoscale devices used in data storage, nanoswitches and biological sensors, due to their nanometre-scale thickness, high surface-to-volume ratio, and fascinating photocatalytic and optical activities [4]. In the last years, the variable features of colloidal nanocrystals, such as their size-dependent electronic, optical, magnetic, mechanical and chemical properties, which cannot be obtained in their bulk counterparts, have attracted the attention of researchers [5]. In particular, within colloidal semiconductors, metal chalcogenide nanocrystals have been extensively investigated due to their size-dependent photoemission characteristics and quantum confinement effects [6]. Among these nanocrystals, metal oxides have gained a significant role in technology development due to their exceptional skills, which allow exploring new application fields, such as optical, electronic, optoelectronic and biological domains. In particular, the application in which metal oxides have been widely used is chemoresistive gas sensing. The performance of sensors based on metal oxides depends crucially on their dimensions, morphology (Fig. 1), composition and surface activity. Among the several parameters that influence the sensing properties of a metal oxide, the potential barrier at the interface between grains is a major physical quantity [7]. Indeed, in this sense, the broad assortment of one-, two- and three-dimensional metal-oxides nanostructures has been a precious source for gas sensors technology, which owes its constant development to the requirements of physical, chemical and biological detection systems [8-9].

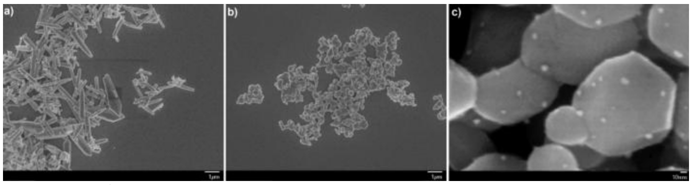

Fig. 1. SEM images of a) nanorods, b) nanoparticles, and c) gold nanoclusters decorated ZnO powders.

However, there are different types of nanostructured materials that may be very good candidates to be further investigated in the chemoresistive gas sensing field, i. e., metal sulfides. Indeed, by using these materials (Cds, SnS_2 in Fig. 2), we expect an improvement from an energy consumption point of view, both in thermal and photo-activation modes, due to their lower band-gap than for metal-oxide semiconductors. This means that the activation of intrinsic surface reactions occurs at lower working temperatures, and then minor power supply is necessary. Due to this advantage, we were motivated in the search for potential improved performance in terms of selectivity and stability. The absence of oxygen in the crystal lattice of metal sulfides leads to a different catalytic mechanism on the surface reaction with respect to metal oxides. In addition, this absence may solve the constant drift of the signal suffered by metal oxides and ascribed to the in/out diffusion of oxygen vacancies, which alters the doping level [10-11].

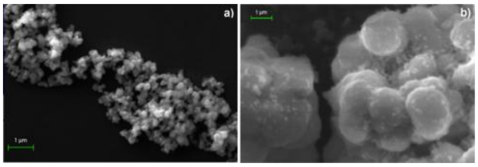

Fig. 2. SEM images of a) CdS, and b) SnS_2 nanopowders.

Recently, organic-inorganic hybrid nanocomposites have quickly gained a prominent position in the gas sensing field. For example, due to its excellent electrical, mechanical and thermal properties chemically modified graphene has been extensively studied as sensing film. So far, the research focused on graphene and graphene-based materials has led to an extensive assortment of highly performing devices, including Functionalized Graphene Oxide (FGO) and its reduced counterpart (rFGO). Modified graphene oxide (GO) has shown good sensing performance, which are critically important to design a commercially viable gas sensing system. In this advent, several approaches are employed to improve the interactions between FGO layer and the gaseous molecules.

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Thursday 31 VIII

A 1D-0D model for the simulation of the cerebral and extra-cerebral flows and pressures

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We developed a 1D-0D model for the simulation of the cerebral and extra-cerebral flows and pressures in humans. It is composed by a comprehensive 1D model of the arterial circulation [1] [2], and two 0D models of the cerebral and brain drainage vasculature [3] [4]. Through a system of differential equations, the model takes into account the pulse-wave transmission properties of the 55 main arteries, together with the principal hydraulic mechanisms that ensure the proper blood supply and drainage of the brain. Pressure results from the arterial 1D model are used as input to the 0D models to simulate several pressure variations due to periodic perturbations like heartbeat, body movements, and the occurrence of vascular diseases like tachycardia. The contribution to venous pressure due to respiration is also added to simulate the effect of the thoracic pump on the drainage system. First results show that the system of equations is stable from the mathematical point of view, without any kind of divergent solution. Moreover, the average behavior of simulated flows is in agreement with experimental data. The model allows to predict changes of important clinical parameters such as venous sinuses pressure, before and after the change of posture or the onset of stenotic patterns.

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Thursday 31 VIII – Invited Lecture

Softening of spin waves calculated under a Hamiltonian approach: importance in information delivery, and in the understanding of reversal avalanches in macrospin networks

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Spin waves (SWs) have became the subject of an intense theoretical and experimental investigation due to their potentiality as dissipationless information carriers for spintronic logic gates and waveguides. Differently from the Fourier analysis of a system's magnetic response after proper excitation, the Hamiltonian approach [1] allows the computation of the whole set of SW modes, independently of the excitation symmetry and action, as an eigenvalue/eigenvector problem; moreover, the modes can be in principle computed arbitrarily close to the critical field for any magnetization change ("transition"), e.g. magnetization reversal, vortex-to saturation transition, etc. The last property is particularly suitable to the calculation of soft modes [2], i.e. SWs with a frequency going to zero at the critical field: at the critical field, this modes are known to trigger the transition by transferring their symmetry to the static magnetization, determining a specific instability that leads the system to reconfigure in a different way. Besides the theoretical interest in describing many kind of changes of the magnetization configuration, soft modes have surprising properties of great importance for spintronics, as a asymmetric broadening of their bandwidth [3] (with different group velocity in different directions), and for a dynamic explanation of the complexity of reversal avalanches (Dirac strings) in macrospin networks like artificial quasicrystals and artificial spin ices [4].

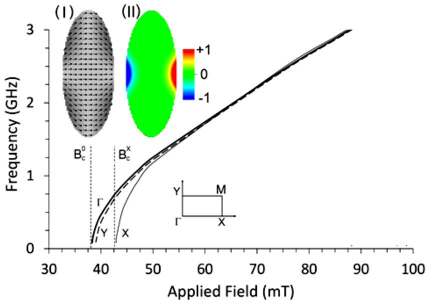

Fig. 1. Softening of a SW 'end mode' (inset II), in a rectangular lattice of saturated elliptical dots (inset I), showing a specific dependence on the Bloch wavevector direction: approaching the critical field (from high values) a frequency band opens for SW propagation along the applied field direction.

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Thursday 31 VIII – Invited Lecture

Nanoscale control of spin wave dynamics in ferromagnetic films

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Spin waves in ferromagnetic thin films span a broad range of frequencies from hundreds of MHz up to tens of GHz with the respective wavelengths ranging from micrometers to nanometers. The spin wave spectrum depends on the magnetization configuration and can be tuned by the external magnetic field. This offers suitable characteristics important for applications in microwave and information processing technology [1]. We present our advances allowing for tailoring of the spin wave dynamics in ferromagnetic thin films by periodic and aperiodic pattern in nanoscale [2, 3, 4]. We explain formation of the spin wave band structure in magnonic crystals, with and without inversion symmetry. Opening of the magnonic band gaps and variation of the band structure resulting from changes of the magnonic crystal geometry and symmetry is exemplified. We show also that the formation of the band structure in a homogeneous magnetic film can be induced by dynamic magnetostatic interactions with the metallic nonmagnetic or ferromagnetic array of stripes placed above the film [5]. This non-invasive formation of the magnonic band structure creates opportunity for exploitation of the nonreciprocal properties in magnonics. Further, control of spin waves can be achieved by change of the spin wave refractive index in a continuous way [6]. We present the influence of gradual variation of the internal magnetic field on the propagating spin wave beams and demonstrate the basic approach for explanation of the properties of the graded index materials, which could be useful in magnonics.

We acknowledge the financial support from NCN project UMO-2012/07/E/ST3/00538 and the EU Horizon 2020 GA No 644348 (MagIC) and SASPRO Programme (REA Grant Agreement No. 609427, 1244/02/01) co-funded by the Slovak Academy of Sciences.

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Thursday 31 VIII

Spin wave refraction on the interface of uniform and patterned magnetic layers

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Propagation of dipolar spin waves through planar systems is highly anisotropic. The spin waves of the same frequency, propagating in different directions, can differ significantly in wavelength. This anisotropic relation between wave vector (wavelength) and frequency of spin waves leads also to an unusual (i.e. not present in isotropic medium) relation between direction of phase velocity and group velocity. The later relation is responsible for refractive properties of the system [1]. The anisotropy of the propagation can be additionally shaped by the introduction of periodic patterning which leads to the folding of dispersion relation into the first Brillouin zone. This effect is already exploited for photonic crystals [2].

We investigated the refraction (and reflection) of spin waves on the interface between two magnetic layers. The interface splits the system into two half-planes (of the same thickness), each characterised by different dispersion relation. We considered uniform (half)planes and patterned (half)planes (in the form of antidot lattices and bi-component magnonic crystals). The following effects were discussed: *angular filtering* (spin wave has to incident at the interface in specific ranges of the angles in order to be refracted), *all-angle collimation* [3] (spin wave is refracted at the direction normal to the interface, regardless of the incidence angle) and *refraction-less transmission* (refraction angle is the same as incidence angle in specific range). All of the mentioned effects can be controlled by the change of the direction of an in-plain applied magnetic field.

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We acknowledge the financial support from NCN project UMO-2016/21/B/ST3/00452 and the EU Horizon 2020 GA No 644348 (MagIC).

Thursday 31 VIII

Short Heisenberg magnets - an insight into the two spin deviations sector

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Heisenberg magnets with spin-1/2, in the two-magnon sector has been examined with the use of several approaches, describing the eigenproblem for the finite case. We start with Bethe equations (BE), which enable to evaluate parameters, that label eigenstates of a magnet, however to find appropriate sets of winding numbers, which parametrize BE, one has to apply the TQ Baxter equation, combined with the Inverse Bethe Ansatz method, or a combinatoric approach, with the use of rigged string configurations. The latter appears to be a tool which ensures the completeness of solutions, and, at the same time, riggings enable to indicate precise winding numbers, so that one can obtain all parameters describing eigenfunctions.

Dynamic magnetic properties of the ferromagnetic quasi 1D ising system $[Co(NCS)_2L_2]_n$; L=pyrydin

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$[Co(NCS)_2L_2]_n$ (L – pyridine) is composed of ferromagnetic chains of Co(II) ions linked by the two NCS bridges. The coordination polyhedron of the Co(II) ion is a distorted octahedron built from equatorial two N and two S and two apical N atoms of the organic ligands. Specific heat and magnetic study showed that $[Co(NCS)_2pyrydine_2]_n$ undergoes a phase transition to the ferromagnetic state at the Curie point of 3.7 K. Magnetic interactions have been determined on the base of the Ising model resulting in the value of the intrachain exchange coupling J/k_B=27 K ($H=Js_is_j$). By means of AC magnetic susceptibility measurements the magnetic relaxations were investigated. Using High Field-High Frequency ESR (HF-ESR) method the magnetic excitations were observed and explained in the frame of the Ising model in accordance with magnetic studies. Energy barriers for magnetization reversal obtained from magnetic and HF-ESR measurements are compared and discussed.

Acknowledgments:

This project was supported by the Deutsche Forschungsgemeinschaft (Project No. Na 720/5-1) and the State of Schleswig-Holstein. We thank Prof. Dr. Wolfgang Bensch for the access to his experimental facilities. ZT thanks the National Science Centre Poland for financial support granted under decision DEC-2013/11/B/ST3/03799. We thank the URZ of the FSU Jena for providing additional computational resources.

Thursday 31 VIII

Study of Bi properties on polymer substrate: a route toward flexible magnetic sensor

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Despite the extensive studies of magnetotransport properties and magnetic phenomena in single material thin films, some of them are still objects of great interest for spintronics technology. Semi-metallic bismuth with its unique features reveals high magnetoresistance (MR) and strong Hall effect even at room temperature. Furthermore, at higher magnetic fields the MR of bulk Bi is larger than that of multilayers exhibiting GMR effect. It is possible because of much lower electron effective mass of bismuth in comparison to other metals. It results in electron mean free path (λ) of the order of micrometers which is lower only than λ of graphene. These properties can be used in design and fabrication of magnetic field sensors.

This contribution describes modification of Bi thin film structure and its influence on magnetotransport properties. Thin bismuth films with different thicknesses were prepared on kapton substrates by thermal evaporation at ultrahigh vacuum. Then the films were annealed in high vacuum in the temperature range from RT to melting temperature. The film morphology and crystallographic structure were studied with scanning electron microscopy (SEM) and X-ray diffraction. The transport properties (magnetoresistance and Hall effect) were measured with standard four-point probe technique at magnetic fields up to 20 kOe. Low-temperature magnetoresistance measurements were carried out at field up to 70kOe and temperature down to 5K.

The temperature dependent XRD measurements allowed to determine the temperature at which the film loses the continuity and the process of dewetting is initiated. This measurements showed at higher annealing temperature grain recrystallization accompanied by grain sizes growth, confirmed also by SEM images. The increase of grain sizes resulted in the significant increase of the magneto- and Hall-resistance due to the lower defect concentration. Both effects showed opposite Bi thickness dependence; the magnetoresistance value saturaterd for thicker films while Hall resistance reached the higher value for film thicknesses close to discontinuity threshold. These properties are beneficial for construction of flexible magnetic field and strain sensors.

Our research of the magnetotransport properties of bismuth layers deposited on polymeric substrates [1] opens the path for applications in flexible electronics. However, development of elastic magnetic sensors requires consideration of several phenomena that are of minor importance in case of rigid bulk materials. Due to the fact that the metalic layer is subjected to unsteady mechanical stresses, deposition of the magnetic sensor onto 12μm thick non-rigid substrate creates a numerous problems, and the strain sensitivity is the first effect which have to be discussed. The thermoelectric effect is the second effect that also have to be considered in order to minimize thermal errors. These aspects will be discussed more detailed in this contribution.

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Acknowlegements
This work was supported by the National Centre for Research and Development within LIDER V program, Poland (project Nr.: LIDER/008/177/L-5/13/NCBR/2014).

Magnetic transition from dot to antidot regime in large area arrays with perpendicular magnetization

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The understanding how the patterning affects the magnetic phenomena and magnetic reversal is an important topic for magnetic recording media, sensors and actuators built as nanostructures on patterned substrates. This work studies the transition between two different magnetization reversal mechanisms for thin Co/Pd multilayers with perpendicular magnetic anisotropy, appearing in magnetic dot and antidot arrays, which were prepared by nanosphere lithography. Various ordered arrays of nanostuctures (see Fig. 1), both magnetic dots and antidots, were created by varying size and distance between the nanospheres employing RF-plasma etching. We have shown that the coercivity values reach a maximum for the array of antidots with a separation length close to the domain wall width. In this case, each area between three adjacent holes corresponds to a single domain configuration, which can be switched individually. On the contrary, small hole sizes and large volume of material between them results in domain wall propagation throughout the system accompanied by strong domain wall pinning at the holes. We have also shown the impact of edge effects on the magnetic anisotropy energy.

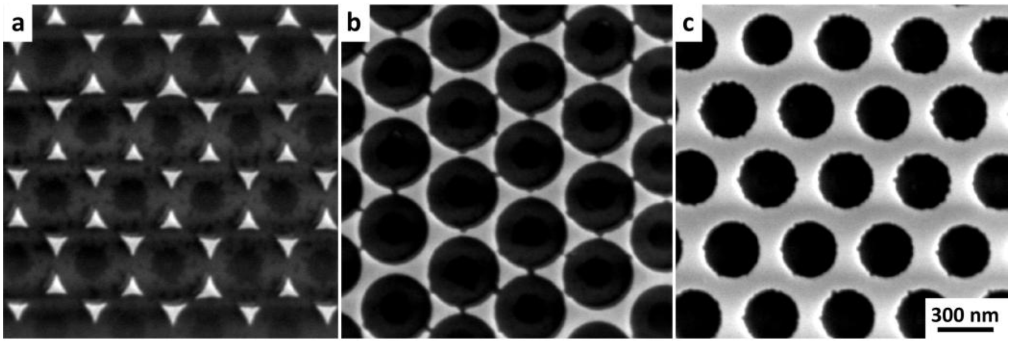

Fig. 1. Scanning electron image of Co/Pd arrays with period of 438 nm. Coverage of the sample surface with magnetic material changes and amounts to (a) 7%, (b) 16% and (c) 55%, resulting in different morphology from separated magnetic islands (a) to arrays of antidots (c).

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ABSTRACTS

Posters

Poster no. 1

High dielectric response in rhombohedral phase of $BaTiO_3$ single crystals

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Unusual increase of the dielectric permittivity of $BaTiO_3$ single crystal in its rhombohedral phase [1] has been a subject of a substantial interest. This effect was related to the appearance of nano-sized domains below 190 K [2] under a suitable electric field pre-treatment.

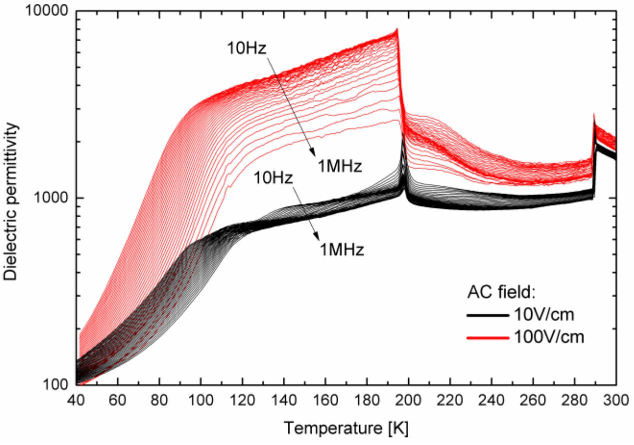

Fig. 1. Temperature dependence of dielectric permittivity of <111> oriented $BaTiO_3$ single crystal at two different measuring signals (10V/cm ad 100V/cm) in frequency range from 10Hz to 1MHz.

Here we report additional insights in the dynamics of this remarkable phenomenon. In particular, we have elucidated the role and the influence of the dc and ac electric field on <111> oriented $BaTiO_3$ single-crystal in the rhombohedral phase. It is shown that the effect of the dielectric permittivity increase is strongly connected with the probing ac voltage (Fig.1) while it does not depend on the dc electric field value. In addition, the frequency dependence has been studied in details within the 10 Hz to 1MHz range and for various amplitudes of the ac field. We also discuss the contribution of ferroelastic domain walls motion and defects to the dielectric response of such a system.

This work was supported by the Czech Science Foundation (Project GACR 13-15110S)

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Poster no. 2

Orientation of the electric field gradient and ellipticity of the magnetic cycloid in multiferroic $BiFeO_3$

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A contribution deals with the hyperfine interactions observed on the ^{57}Fe nucleus in multiferroic $BiFeO_3$ by means of the 14.41-keV resonant transition in ^{57}Fe, and for transmission geometry applied to the random powder sample. Spectra were obtained at 80 K, 190 K and at room temperature. It was found that iron occurs in the high spin trivalent state. Hyperfine magnetic field follows distribution due to the elliptic-like distortion of the magnetic cycloid generated by the Dzyaloshynskii-Moriya interaction. The long axis of the ellipse is oriented along $\langle 111 \rangle$ direction of the rhombohedral unit cell. The hyperfine magnetic field in this direction is about 1.013 of the field in the perpendicular direction at room temperature. This ratio diminishes to 1.010 at 80 K. Axially symmetric electric field gradient (EFG) on the iron atoms has the principal axis oriented in the same direction and the main component of the EFG is positive. Our results are consistent with the finding that iron magnetic moments are confined to the $[1\bar{2}1]$ crystal plane. Figure 1 shows probability density $\rho(B)$ of apparent distribution of the hyperfine field B due to the magnetic cycloid deformation at various temperatures [1].

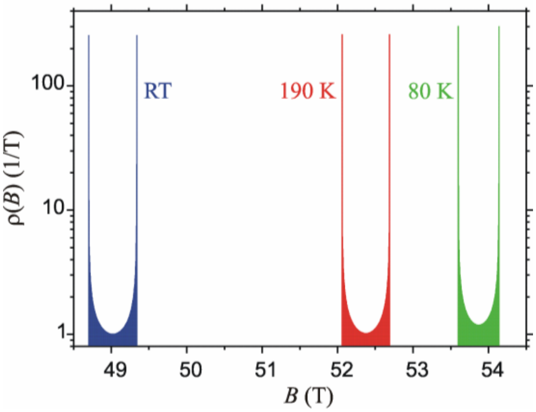

Figure 1 Probability density of apparent field distribution plotted versus hyperfine field B for three different temperatures [1].

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Poster no. 3

Magnetic relaxations in trinuclear complex [TbIII(ZnIIL)2]CF3SO3 induced by applied static magnetic field

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Examined compound [TbIII(ZnIIL)2]CF3SO3 is a Single Molecule Magnet (SMM) which crystalize in trigonal system with space group R32 (a = b = 11.8682(4) Å, c = 38.4392(16) Å) and does not exhibit any phase transition to a long range magnetically ordered state in the temperature range of 2 K to 300 K. At room temperature (300 K) χT value was estimated as 13.04 (emu·K)/mol and was larger than expected 11.81 (emu·K)/mol. The temperature dependence of χT may attribute to the thermal depopulation between sub-levels of ground multiplet of TbIII ions due to magnetic anisotropy. Samples had a shape of flattened disc as it is showed in a Figure 1. Magnetic properties of crystalline sample were carried out as a function of sample orientation in a regard to applied external magnetic field. Magnetic relaxations shows strong dependence of static magnetic field and are well described by generalized Debye model with one relaxation time and narrow distribution.

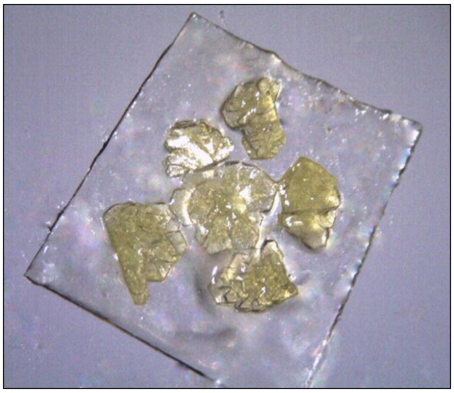

Figure1. Picture of measured sample.

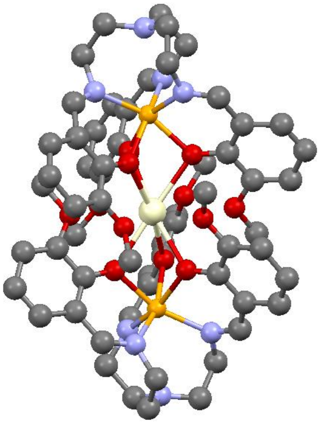

Figure 2. Structure of one [$Tb^{III}(Zn^{II}L)_2$]CF_3SO_3 cluster. Molecules of hydrogen were omitted for clarity of picture.

Poster no. 4

A-D-A-type 9,10-bis(phenylethynyl)anthracenes (BPEAs) for small molecule organic solar cells

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Fossils fuels are slowly running out and they are also problematic in terms of environmental issues. Therefore, the alternatives of coal, petrol and gas are intensively explored, such as solar energy for instance. Organic photovoltaic systems seems to be a good choice to fulfill the criteria of safe and efficient source of cheap energy. Organic π-conjugated materials as active materials can be easily prepared in bulk quantities and large area devices can be fabricated by the solution process compared to silicon and germanium. One of the most interesting classes of compounds is acetylenes [1]. The main reason of triple bond chemistry booming is the availability of efficient protocols for palladium catalyzed alkynylation reactions [2,3]. Below we present the photovoltaic activity of A-D-A (acceptor-donor-acceptor) type 9,10-bis(phenylethynyl)anthracenes (BPEAs) in solar cells. The compounds were prepared in four consecutive steps using Sonogashira reaction and Knoevenagel condensation [4,5]. The preliminary study of photovoltaic performance revealed that anthracene based A-D-A molecules shows photovoltaic activity with an average power conversion efficiencies (PCE) of 2.7%.

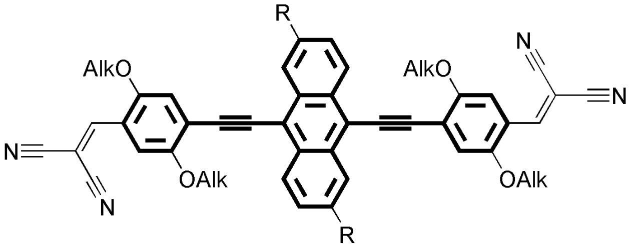

Fig. 1. A-D-A BPEA

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Poster no. 5

Computational study of the vacancy order in 2/1 mullite

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Although mullite ($Al_{4+2x}Si_{2-2x}O_{10-x}[vacancy]_x$) is known since 1924 its crystal structure is still under debate [1]. Recently, a new description of the most ordered state of mullite based on the superspace formalism has been proposed [2]. According to this model, the vacancy distribution can be described as a block structure of vacancy blocks that alternate with vacancy-free blocks (Fig. 1) and the incommensurate nature of mullite originates from a modulation of the block size that depends on the composition.

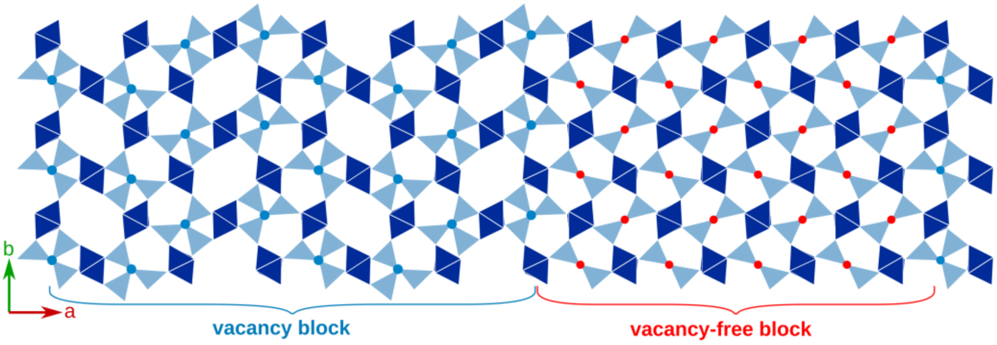

Fig. 1. Scheme of the vacancy distribution

In this work, we present a computational study of the stability and disorder of the model together with a comparison with a previous proposal, which is also based on the ordering of the vacancies in blocks [3] for the 2/1 mullite. We use *ab initi*o calculations to investigate the ground state and classical molecular dynamics simulations to monitor the jumps of vacancies at finite temperatures for both models.

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Poster no. 6

Mössbauer spectroscopy in the studies of sedimentation of Fe_2O_3 in water solution of sugar

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The Mössbauer spectroscopy, traditionally applied for the investigation of the solid state problems may be extended to the studies of dynamics of nanoparticles in suspensions. In particular, the competition between the Brownian motion and gravitational sedimentation may be observed.[1,2] The processes of sedimentation of nanoparticles occur in many technological and natural processes.

In this work we describe the results of the study of the sedimentation hematite submicron particles (fig.1) in concentrated water solution of sugar (sucrose, $C_{12}H_{22}O_{11}$) . After 1-12 days of the fall of hematite in suspension, the samples were taken from five fixed depths. The concentration of nanoparticles in slurry was determined by weighing them before and after drying.

The method of the determination of the mobility of nanoparticles from Mössbauer spectra is based on the Brownian movement theory[3]. Such method has been described previously in water solutions (see Fig.2) and was studied in situ by transmission Mössbauer spectroscopy in horizontal and vertical geometry[4].

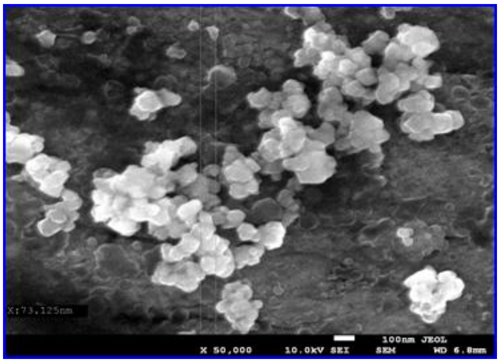

Fig. 1 The 110 nm nanoparticles of hematite from water solution. During evaporation of water the particles are deposited on the surface randomly

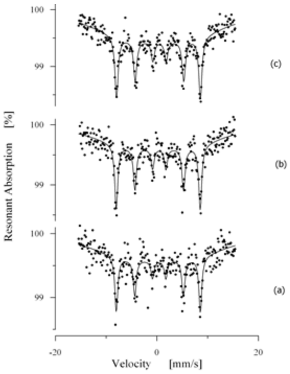

Fig.2 Mössbauer spectra of hematite nanoparticles in water solution measured in vertical geometry together with their sediment, measured after 5 h (a), 50 h (b) and 90 h (c).[4]

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Poster no. 7

Diffuse scattering at ID28 ESRF side station : a new tool for lattice dynamics studies

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We present the specialized diffractometer that was built as a side station of the inelastic x-ray scattering (IXS) beamline ID28. Side station is able to operate in parallel with the IXS station, and is open to users since 2017. Software for data reduction is provided to the users.

The proposed instrument shall be primarily dedicated to the study of diffuse scattering in a large class of materials ranging from strongly correlated electron systems to nanoscale-modulated and low-dimensional systems, and will constitute a powerful tool in the study of lattice dynamics complementing the inelastic x-ray scattering studies. Investigations of a large class of crystalline systems with correlated disorder will greatly benefit from the dedicated station, thanks to a flexible sample environment. The high brilliance of the x-ray source, coupled to state-of-the-art detection schemes, using hybrid pixel detector, will open the window to time-resolved studies and studies under extreme conditions.

The diffuse scattering station in combination with the existing IXS instrument on ID28 constitutes a world-wide unique experimental station, offering unprecedented capabilities in the studies of lattice dynamics in condensed matter and of the real structure of functional materials to the large ESRF user community. A few benchmark systems are presented, as well as a method to obtain the full elasticity tensor from a thermal diffuse scattering experiment [1], based on the example of sulfate crystals.

Fig. 1. Picture of ID28 side station

[1] Wehinger *et al*, Full elasticity tensor from thermal diffuse scattering, PRL 118, 035502, 2017.

Poster no. 8

Phase transitions and molecular dynamics of ionic coordination compounds of the$[M(DMSO)_6](BF_4)_3$ type, where M = V and Fe

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Two ionic coordination compounds with dimethyl sulfoxide (DMSO = $OS(CH_3)_2$) acting as a ligand, $[V(DMSO)_6](BF_4)_3$ and $[Fe(DMSO)_6](BF_4)_3$, have been synthesized and their phase polymorphism has been investigated using differential scanning calorimetry DSC (100–330 K) and Fourier transform infrared absorption spectroscopy FT-IR (13–320 K). Both compounds exhibit orientational dynamical disorder of the $OS(CH_3)_2$ ligands as well as BF_4^- anions across a wide temperature range, and therefore belong to so-called orientationally dynamically disordered crystals (ODDIC).

Four solid-solid phase transitions were detected in both investigated compounds, what indicated the DSC curves obtained during cooling and subsequent heating (see Fig. 1).

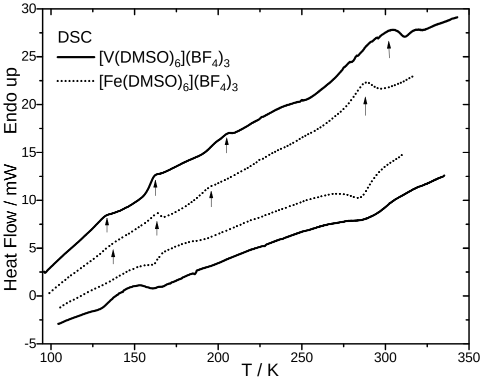

Fig. 1. The DSC curves registered for both compounds with a scanning rate of 25 $Kmin^{-1}$. For clarity the arrows indicate the regions of phase transitions' occurrences during heating.

All the transitions occur between stable phases and their transition temperatures as well as character are very similar for both compounds. In our presentation we will characterize the transitions discovered and discuss their connection to reorientational dynamics and/or structural changes. The polymorphism of the investigated compounds will be also compared with the results obtained for the two other coordination compounds of the same type: $[Cr(DMSO)_6](BF_4)_3$ and $[Al(DMSO)_6](BF_4)_3$ [1-2].

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Poster no. 9

Thermal properties and molecular dynamics of triblock semifluorinated n-alkanes probed by temperature-dependent infrared absorption spectroscopy

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Thermal behavior of a series of semifluorinated long chain alkanes of the general formula: $H(CH_2)_m(CF_2)_6(CH_2)_mH$ (in short $H_mF_6H_m$), where m = 16, 18 and 20, has been previously investigated by differential scanning calorimetry (DSC) and polarized optical microscopy (POM) in temperatures between 245 K and 360 K [1-2]. The results revealed that all three compounds exhibit rich polymorphism including ordered crystalline phases and liquid crystalline (smectic E and smectic B) phases even though these compounds do not possess aromatic core characteristic for liquid crystal materials.

In order to obtained more detailed information on molecular dynamics and/or structural changes occurring at the transitions temperature-dependent Fourier transform middle infrared absorption spectroscopy (FT-MIR) has been applied both upon heating and subsequent cooling. Splitting of some bands and occurrence of new ones at the phase transitions' regions have been observed and interpreted. Also, the temperature behaviors of positions, intensities and full width at half maximum (FWHM) of the bands associated to the vibrations within CF_2 and CH_2 groups have been studied *(see exemplary results in Fig. 1)*. Comprehensive spectroscopic analysis will be presented.

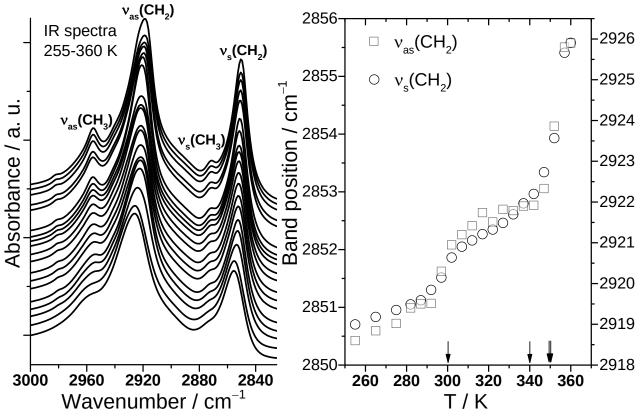

Fig. 1. Temperature evolutions of the FT-MIR spectrum in the range of 3000–2825 cm^{-1} (left) and of positions of the $\nu_{as}(CH_2)$ and $\nu_s(CH_2)$ bands (right) of $H_{20}F_6H_{20}$.

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Poster no. 10

Optimizing acoustic wave – spin wave resonant coupling in the magphonic crystal

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We have investigated co-directional and contra-directional couplings between spin wave and acoustic wave in one-dimensional periodic structure (magphonic crystal). The system consists of two ferromagnetic layers alternating in space. We have taken into consideration materials prominent in magnonics: YIG, CoFeB, permalloy, and cobalt. The coupled mode theory (CMT) formalism have been successfully implemented for the first time to describe magnetoelastic interaction as a periodic perturbation in the magphonic crystal. We have shown, that CMT analysis of magnetoelastic coupling allows to effectively design a spin wave-acoustic wave transducer based on a magphonic crystal. Analitycal results have been compared with frequency-domain and time-domain numerical simulations.

We have demonstrated how the energy is spatially exchanged between spin wave and acoustic wave in the optimized magphonic crystal if the resonance condition is satisfied. In the case of contra-directional coupling, i.e. when spin wave and acoustic wave have opposite signs of the group velocities, we have observed phenomenon similar to the Bragg reflection at the frequency in the stop band However, if the wave that incides to the structure is purely elastic, the reflected wave is purely magnetic. What is more, the reflected spin wave has much shorter wavelength compared to the acoustic wave. On the other hand, in the co-directional coupling, i.e. when spin wave and acoustic wave have the same signs of the group velocities, we have observed complete conversion of energy from spin wave to acoustic wave periodically in space. Since the exchange length is in the micrometer and sub-micrometer scale, such conversion should be experimentally achievable. Moreover, we propose thin film – substrate systems optimized for the experimental investigation of the linear coupling between surface spin waves and surface acoustic waves.

Acknowledgements

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Poster no. 11

High-pressure cells for inelastic neutron scattering studies of proton dynamics in materials

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A specific generation of compact high-pressure cells is developed for experiments on inelastic neutron scattering. The cells of a generic “piston-cylinder” type offer a pressure range up to 30 kbar with the sample volumes up to 100 mm^3. The cell body may be composed from different metallic alloys such as Cu-Be, Ti-Zr, Ni-Cr-Al or their combination. The energy of atomic vibrations in these materials does not exceed some 40-45 meV what permits studies of higher energy excitations, including proton vibrations in different compounds, in relatively comfortable experimental background conditions. The cell design is particularly adapted for the neutron spectrometer IN1-Lagrange at ILL with large open solid angle for scattered neutrons. The performance of the first members of this high-pressure cell family is illustrated by the phonon spectra measured on IN1.

Poster no. 12

Not so giant anharmonicity in PbTe

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The problem of anharmonicity in crystals is a long-standing issue in solid state physics. And it is an important one. Nevertheless it does not necessairly warrant sansational headlines in the high-end scientific journals [1]. In this presentation, we show that in the case of PbTe the automatic claim of strong anharmonic effects as a default suspect for any unexplained lattice dynamics phenomenon may not be entairly correct. Furthermore, in light of recent published results [2] and presented calculations the case may be even more complicated than naiively expected.

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Poster no. 13

Phase behaviour of banana-shaped molecules confined between walls

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We investigate the stabilization of liquid crystalline structures in a three-dimensional system of banana-shaped molecules. Our work [1] is a generalization of studies concerning recently discovered nematic splay-bend phase [2]. Using Density Functional Theory, Monte Carlo and Molecular Dynamics simulations we analyze system of banana-shaped molecules composed of connected spheres interacting via hard-sphere or the repulsive part of the Weeks-Chandler-Andersen (WCA) [3] potential. In addition to the previous studies, we introduce interaction with two parallel walls, which can greatly influence phase behaviour of the inner system in their vicinity. We present the differences of the near wall and bulk properties of analyzed molecular systems.

Acknowledgments

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Poster no. 14

Molecular dynamics in the antiferroelectric liquid crystal (2S)-octano-2-yl4'-(2-fluoro-4-{[5-(1,1,2,2,3,3,3 heptafluoropropoxy)pentylo]oxy}benzoyloxy)-[1,1'-biphenyl]-4-carboxylate

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The complex of polymorphism and molecular dynamics of (2S)-octano-2-yl4'-(2-fluoro-4-{[5-(1,1,2,2,3,3,3 heptafluoropropoxy)pentylo]oxy}benzoyloxy)-[1,1'-biphenyl]-4-carboxylate, abbreviated as 2F5, have been studied by complementary methods i.e. differential scanning calorimetry (DSC), polarizing microscopy observations and broadband dielectric spectroscopy (BDS). 2F5 is built of chiral molecules and shows rich polymorphism of liquid-crystalline and solid phases. Studies by DSC and polarizing microscopy methods revealed the following phase sequence: SmA*, ferroelectric SmC*, antiferroelectric SmC*$_A$ and the glassy GSmC*$_A$ phase. Additionally, on slowly heating (< 1,5 K/min) a „cold crystallization" was observed. Phase transitions between particular liquid-crystalline, glassy and crystalline phases were confirmed by the alteration in the temperature dependence of the dielectric spectra. In frequency range from 0.1 Hz to 3 MHz the relaxation processes were detected in liquid-crystalline smectic phases. The processes observed in SmA* and SmC* phases were identified as a soft mode and Goldstone mode respectively. Two relaxation processes (s-process and ferroelectric amplitudon) were detected in antiferroelectric SmC*$_A$ phase. Mechanism of complex dynamics (molecular and collective) of smectic phases was identified with help of the bias field.

Acknowledgements

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Poster no. 15

Applications of colorants in OLEDs and photovoltaics

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Organic light-emitting diodes (OLEDs), are area light sources, that contains active layers thinner than 500nm. Organic solar cells, are types of photovoltaics, that consist of conductive organic materials. The crucial factor in engineering OLEDs and organic solar cells, is selection of materials for electrodes, and polymers for active layers. The use of organic fluorescent or phosphorescent colorants in both OLEDs and organic solar cells might provide new, interesting possibilities as they influence performance characteristics. Presented OLEDs and organic solar cells were built with ITO/PEDOT:PSS/active layer/(Ca/Al) architecture [1]. Active layers consisted of one organic compound with or without a dye, or consisted of a mixture of two to three organic compounds. Commercially available colorants (Uvitex) and non-commercial colorants (AP3, AP4, AP5) were used in the research. As organic compounds for active layers were mainly used polymers such as: PVK (poly(9-vinylcarbazole)) [2], P3OT (poly(3-octylthiophene-2,5-diyl)) [3] and P3HT (poly(3-hexylthiophene-2,5-diyl) [1]. The results of tests conducted on obtained organic solar cells and OLEDs will be further presented.

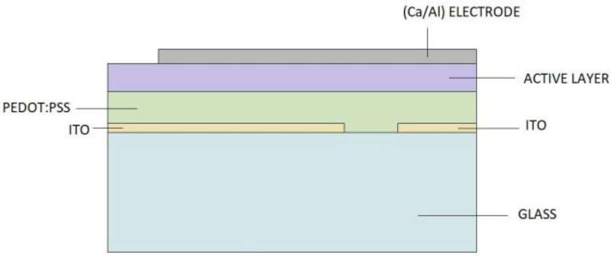

Fig. 1. Scheme of the OLEDs and organic solar cells architecture

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Poster no. 16

Measurement efficiency of Second Harmonic Generation (SHG) with consideration reflected signals

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Principal set-up for measurement of higher harmonics of light is presented in Fig. 1. In left diagram of Fig. 1 is typical measuring system for second harmonic generation [1]. Consideration of first and second harmonics in this system depends on probe efficiency and detectors position. Changing detector's location will influence of measurement result.

The modified measurement method (right diagram Fig. 1) is supported measurements of opaque and powder probes where it is not possible to measure the second harmonic after passing through the crystal. It gives the opportunity to estimate and separate microscopic and macroscopic susceptibility [2, 3], which is principal for characteristics of condensed matter.

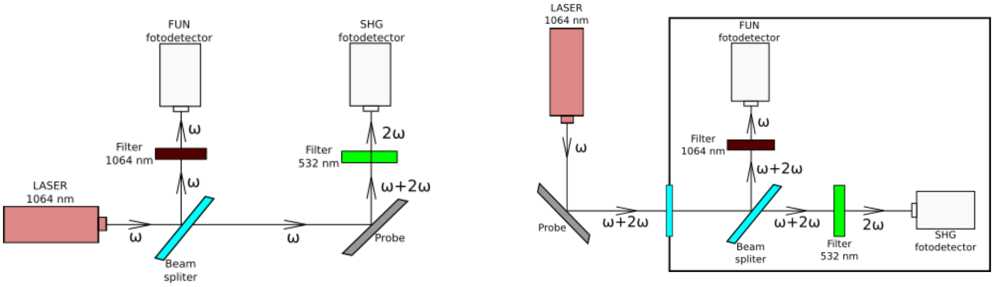

Fig. 1. Typical measurement method (left diagram), modified measurement method (right diagram)

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Poster no. 17

Quantum entanglement in double quantum well-, double quantum wire -structures and Jaynes-Cummings model

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In this work we proposed a new approach to producing the qubits in electron transport in low-dimensional structures such as double quantum wells or double quantum wires (DQW). The qubit could arise as a result of quantum entanglement of two specific states of electrons in DQW-structure. These two specific states are the symmetric and antisymmetric (with respect to inversion symmetry) states arising due to tunneling across the structure, while entanglement could be produced and controlled by means of the source of non-classical light. We examined the possibility to produce quantum entanglement in the framework of Jaynes-Cummings model and have shown that at least in principle, the entanglement can be achieved due to series of 'revivals' and 'collapses' in the population inversion due to the interaction of a quantized single-mode EM-field with a two-level system.

Poster no. 18

Formamidinium Iodide: insight into thermal, electrical and spectroscopic properties

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Recently, small-molecular-weight organic single- and two-component polar materials have developed as a promising candidate in capacitors and in piezoelectric, pyroelectric, and electrooptical devices. Their nonlinear characteristics have been found to be very useful, for example, in optical second-harmonic generators and other nonlinear optical components [1]. Among them, a special interest has been recently paid on iodide compounds and their significance in modern photovoltaic technologies.

Following the discovery of several organolead trihalide solar cells [2] based on formamidinium (FA) cation and despite of many studies on FA-based perovskite structures we have found that the physicochemical properties of the main precursor, formamidinium iodide (FAI) has not yet been well recognized. Based on results presented by Petrov *et. al.* [3] it appears that FAI undergoes two reversible phase transitions at about 346 and 387 K and adopts monoclinic symmetry (space group $P2_1/c$) in the room temperature phase. The X-ray powder diffraction data collected at different temperatures confirm the existence of orthorhombic and cubic phases at 358 K and 400 K, respectively. In this poster, the synthesis, thermal and dielectric properties are presented. To throw more light on the molecular mechanism of the high temperature phase transitions the infrared and ^{1}H NMR studies were carried out in a wide temperature range.

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Poster no. 19

Heliconical and other modulated nematic liquid crystals within Landau–de Gennes description

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Understanding structural properties of recently discovered modulated nematic phase is very topical issue among current liquid crystals research subjects. This phase is heliconical twist–bend nematic (N_{TB}), where the main director lies on the cone and rotates along the wave vector. The influence of the external fields on the N_{TB} phase is the most unexplored research, experimentally showing the shift of the temperature transition from N_{TB} phase to uniform nematic phase [1, 2], and with theoretical description attempts [see for example: 3, 4, 5] on the basis of the Frank elastic theory. Here we explore in depth the Landau–de Gennes theory of the modulated nematics [6–9] to analyze mechanisms of spontaneous chiral symmetry breaking in these materials.

In this presentation we study the bifurcation analysis and numerical minimization within the helicity mode expansion of full free energy. We found number of nematic structures with one–dimensional periodicity, where one of them is the N_{TB} phase. Those structures comprise: nonchiral transverse and longitudinal polarization waves, the splay–bend (N_{SB}) phase with its chiral counterpart. The results provide detailed identification of modulated phases and are also gathered in the form of phase diagrams showing phase transitions among uniform and modulated nematics. In addition, assuming that N_{TB} phase is described only by steric dipoles we investigate the behavior of this structure in an external uniform field. Here the analysis is performed in two ways: minimization of the helicity mode expansion and the relaxation method of a full free energy. Systems with positive dielectric anisotropy exhibit unwinding of the N_{TB} phase to the nematic phases. The filed–induced transition between N_{TB} and N_{SB} phases occurs in the case of negative dielectric anisotropy, where the intermediate elliptic N_{TB} phase is present. This transition is realized by flattening the twist–bend cone, where the axis of the phase modulation is perpendicular to the direction of the applied external field, and where for strong fields the polarization vector acquires the uniform component along this field leading to polar nematic phases.

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Poster no. 20

Raman scattering investigations of phase transitions in the nanocrystals of $PbZrO_3$-$BiFeO_3$ system

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Recently, the origin of antiferroelectricity is widely discussed in literature. Basing on the lattice dynamics in $PbZrO_3$ a phenomenological model with competing interactions between AFE and FE modes was proposed by Tagantsev [1]. It is well know that competing interactions can be strengthened by doping or pressure. Consequently some chemical modifications by different cation replacement can strengthen either FE mode (i.e. Ti4+) or AFE mode (i.e. Sn4+) . Form the available literature it is known that doping of $PbZrO_3$ with $BiFeO_3$ less than 20% does not alter the parent orthorhombic structure of PbZrO3 [2]. $PbZrO_3$ is as classical antiferroelectric with *Pbam* orhorhombic space group [1] whereas $BiFeO_3$ is known as multiferroic possessing rohombohedral *R3m* structure [3]. Such a system system has received some interest in the past [2] primarily due to investigation of the Mössbauer effect which were aimed to solve the problem of the soft mode existence in antiferroelectric crystal [4].

Here we reinvestigate the phase transitions sequence of $PbZrO_3$ substituted with small amount (4%) of $BiFeO_3$ by means of, micro-Raman scattering, dielectric and differential scanning calorimetry (DSC) measurements. Our measurements confirmed that this solid solution undergo two phase transitions within the approximate temperature range 450-500K and about 600K, in agreement with previous findings [2]. Both phase transitions are undoubtedly of first-order character. On the basis of Raman spectroscopy, the symmetry of lower temperature phase was found to be the same as in pure $PbZrO_3$, whereas the intermediate phase of PZO-4$BiFeO_3$ is similar to the antiferroelectric intermediate phase of $Pb(Zr_{1-x}Sn_x)O_3$ solid solution [5]. In next step we will try to explain the mechanisms of the phase transitions existing in the compound with special emphasis for searching of the potential soft mode (or soft modes).

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Poster no. 21

Magnetic Lifshitz transition in multi-band iron-based superconductors

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In this lecture we address Lifshitz transition induced by applied external magnetic field in a case of iron-based superconductors, in which a difference between the Fermi level and the edges of the bands is relatively small [1]. We introduce and investigate a two-band model with intra-band pairing in the relevant parameters regime to address a generic behavior of a system with hole-like and electron-like bands in external magnetic field [2]. Our results show that two Lifshitz transitions can develop in analyzed systems and the first one occurs in the superconducting phase and takes place at approximately constant magnetic field. The chosen sets of the model parameters can describe characteristic band structure of iron-based superconductors and thus the obtained results can explain the experimental observations in FeSe and Co-doped $BaFe_2As_2$ compounds. We also discuss this behavior in the aspect of the ultra-cold fermion gases [3].

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Poster no. 22

Permittivity of polycrystal – laminar structure

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Effective properties (dielectric, magnetic, mechanical) of inhomogeneous materials are important for applications and so it is very desirable to determine them from given known microstructural parameters and from the bulk properties of homogeneous components. The inhomogeneities can be realized in many ways for example by random arrangements of anisotropic grains of polycrystal material or ceramics and their theoretical description is usually rather complex task [1]. Depending on the system various effective medium models are used for interpretation of experimental measurements. The dielectric response is often described by the well-known mixing rules such as Wiener, Maxwell-Garnett, Bruggeman, Hashin-Shtrikman, Lichtenecker or logarithmic, among which the last two are essentially empirical [2]. The 2-component composites and uniaxial polycrystals (ceramics) can be also modeled within the general concept of the Bergman spectral representation [2] together with the numerical simulations, e. g., the finite element method [3, 4]. Even more complicated situation occurs in the strongly dispersive materials, where the dielectric spectrum cover broad frequency range (e. g. 10^2 – 10^{13}Hz in perovskite $Pb(Mg_{1/3}Nb_{2/3})O_3$ ceramics [4]), where the surface plasmons play an important role.

In this contribution a simple model of the polycrystal is constructed that can be solved analytically and provides various mixing formulas. The laminar polycrystal (or polydomain [5, 6]) structure is considered, the layers of which are rotated anisotropic crystallites. The effective dielectric response of such structure is much complex comparing with the layered structure built up of the isotropic materials. The latter serves either parallel or serial capacities only, depending on the direction of the electric field. In case of the polycrystal the effective permittivity tensor depends on the particular distribution of crystallite orientations. Several distributions are analyzed, and in particular, a distribution of orientations is found that results in the exact logarithmic mixing law: $\log \varepsilon_{\mathrm{eff}} = x \log \varepsilon_1 + (1-x) \log \varepsilon_2$, x is the volume fraction. The random uniform 2D rotations of crystallites about an axis and the rotations in the 3D space are considered, and the percolation phenomena and the macroscopic symmetry are discussed.

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Poster no. 23

Comparative broadband dielectric spectroscopy studies of relaxor and non-relaxor $PbFe_{1/2}Ta_{1/2}O_3$ ceramics

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$PbFe_{1/2}Ta_{1/2}O_3$ (PFT) belongs to a rich family of double perovskites $Pb(M'^{3+}_{1/2}M''^{5+}_{1/2})O_3$ with M'=Fe,Sc,In,Yb, and M"=Nb,Ta,Sb. In these compounds, M'^{3+} and M''^{5+} cation positions may be either ordered or disordered. As a rule in the ordered state these perovskites have non-diffused ferroelectric or antiferroelectric phase transitions while in the disordered state they exhibit a relaxor behavior [1]. Recently we found out [2] that in contrast to PFT single crystals [3] and ceramics obtained by a routine solid state reaction route [4,5], PFT ceramics sintered from mechanoactivated powders do not show relaxor properties in the 10^2–10^6 Hz frequency range even though Fe and Ta cations are chemically disordered [6].

In the present contribution, complex dielectric permittivity of both relaxor and non-relaxor PFT ceramics was studied in the low-frequency (1 Hz–1 MHz), microwave (1 MHz–1.8 GHz), THz (100–500 GHz) and infrared (1–100 THz) regions. PFT undergoes phase transitions from the cubic paraelectric ($Pm\bar{3}m$) to tetragonal ferroelectric ($P4mm$) phase at T_{C1} = 240–270 K, and then to the monoclinic ferroelectric (Cm) phase at T_{C2} = 200–220 K [7]. Both ferroelectric phase transitions are revealed in the temperature changes of permittivity, pyroelectric current and polarization hysteresis loops.

THz and far IR studies revealed qualitatively similar temperature dependences of phonons in ferroelectric and relaxor ferroelectric PFT. The soft mode is split at all temperatures and exhibits a minimum near T_{C1}. Lower-frequency component is overdamped at all temperatures, the higher-frequency one is heavily damped but sharpens on cooling below T_{C1}. The behavior of all these phonons reminds canonical relaxors like PMN [8]. Two additional dielectric relaxations can be seen in microwave and radio-frequency ranges. Their temperature evolution will be discussed in detail.

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Poster no. 24

The phonon density of states and magnetic properties of bis-2-phenylethylamine-CuCl$_4$, -MnCl$_4$ and their mixed crystals

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Due to their crystal structure the bis-2-phenylethylamine-CuCl$_4$, -MnCl$_4$ (PEA-CuCl$_4$ and PEA-MnCl$_4$) and their mixed crystals provide interesting systems for thermoelectric applications. The structure consists of MCl$_6$ corner-sharing octahedra (with M = Cu, Mn) which form 2D-layers separated by organic molecules[1]. The space group of both compounds is Pbca at ambient conditions. The thermoelectric figure of merit is essentially determined by the competing effects of the electric and thermal conductivities. While the former is almost confined to the electronic properties of the inorganic layers, the latter is determined by the propagation of phonons. The large organic spacer molecules are supposed to act as efficient damping elements that reduce the thermal conductivity. Moreover, it is expected that the thermoelectric performance can be improved by the substitution of the transition metals. Furthermore these compounds show interesting magnetic properties. The Copper derivative is ferromagnetic and the manganese derivative is antiferromagnetic [2]. Also confirmed by SQUID measurements of the corresponding powder samples.

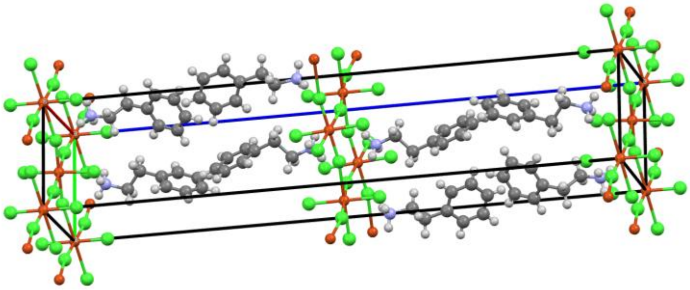

Fig. 1: Crystal Structure of (PEA)$_2$MCl$_4$, M = Cu, Mn

We report on phonon investigations of PEA-CuCl$_4$ and PEA-MnCl$_4$ which help to understand the basic mechanisms of the thermal conductivity. First Raman-results obtained from large single crystals are presented which provide information of low lying Gamma-point optical modes. Moreover, the phonon density of states is obtained by incoherent neutron scattering from hydrogen atoms of the organic spacer molecules in powder samples using the Time-of-Flight spectrometer at the FRM 2 in Garching/Munich. Furthermore new SQUID measurements and the crystallization procedure of the mixed crystals are presented.

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Poster no. 25

Domain wall symmetry is described by layer groups

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Existence of *macroscopic tensor properties* (e.g., pyroelectricity, piezoelectricity, optical activity, electrooptics) of a homogeneous 3-dimensional medium is determined by its *point group symmetry*. There is a question whether a similar approach to macroscopic properties is applicable to a highly nonhomogeneous domain wall (DW), i.e. whether a meaningful concept of DW symmetry can be introduced. The problem has been approached in two ways:

In **Ginzburg-Landau theory** a DW is represented in the order parameter space by a *path* connecting the *points* representing the first and the second domain state. The symmetry of a DW has been identified with symmetry of a homogeneous 3-*dimensional structure* with 3-*dimensional periodicity* represented by the point on the path corresponding to the centre of the wall [1,2].

In **rigorous crystallographic theory** the *symmetry of DW* is that of associated *domain twin* consisting of two domains connected by a coherent planar interface (DW) forming together a nonhomogeneous *3-dimensional object* with *2-dimensional periodicity* along the planar DW. Then the symmetry of a DW (domain twin) is expressed by a *layer group* [3].

These two approaches provide different DW symmetries as, e.g. shown (Fig.1) in a ferroelastic DW in KSCN with symmetry reduction I4/mcm (parent phase) → Pbmc (ferroelastic phase) [1,4]:

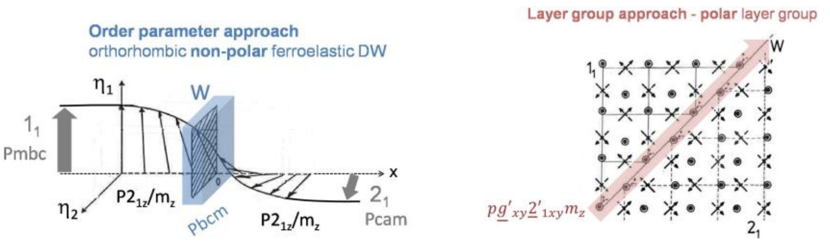

Fig.1 Comparison of two approaches to symmetry of ferroelastic domain wall in KCSN.

We disclose causes of this inconsistency and mention experimental results which support the second approach [5].

Acknowledgments: The present work was supported by the Austrian Science Fund (FWF) Grant No. P28672-N36.

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Poster no. 26

Magnons in the multiferroic phase of cupric oxide

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Cupric oxide (Cu(II)O) has attracted renewed interest over the last years after the existence of a high-temperature multiferroic phase was discovered. Unlike other multiferroics with phase transition temperatures well below 50 K, CuO shows multiferroic behaviour in the incommensurate antiferromagnetic phase between 230 and 213 K. The magnetic structure is characterised by a cycloidal spin arrangement in contrast to the collinear antiferromagnetic low-temperature phase. However, not much is known about the magnetic dynamics of the multiferroic phase, since only magnons at temperatures below 213 K were studied so far.

We therefore present the first spectra of magnons in the multiferroic phase ever observed. In addition to this we also performed comparative measurements in the low-temperature phase. The new polarisation analysis of PUMA@FRMII provides a new, powerful tool for a better understanding of the individual excitations. With this setup, it is possible to detect both spin states of the neutron beam simultaneously. As an example Fig. 1 (left) shows the results of a constant-Q-scan up to 25 meV at the position of the magnetic satellites within the (002) Brillouin zone in the multiferroic phase. The red circles (spin-flipped neutrons) correspond to a magnon polarised perpendicular to the cycloidal plane with a pronounced spin band gap of about 4 meV. This gap is considerably smaller compared to the low-temperature phase (fig.1 right). An additional magnon appears in the modulated phase that is polarised within the cycloidal plane since it is observed in the non-spin flip channel (black squares). Within the experimental resolution it exhibits no sign of a spin gap. This magnon can be attributed to a phason mode of the spin cycloid.

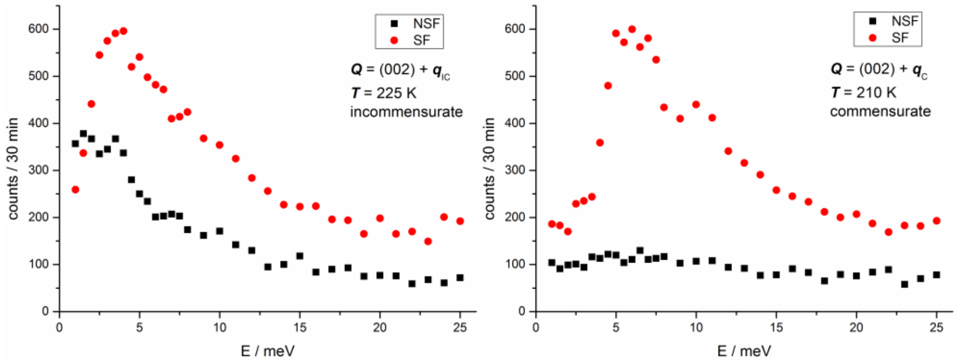

Fig. 1. Constant-Q-scan at the magnetic zone center in the multiferroic (left) and low-temperature phase (right), respectively.

Poster no. 27

Dynamical properties of supercooled water in nanopores

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In the present work we investigate the dynamical properties of supercooled water in the porous glasses Vycor (pore size 10 nm) and Gelsil (pore sizes 2.6 nm and 5 nm). For this investigation we used Perkin Elmer apparatus: Diamond DMA, DMA 8000, DMA 7 and TMA 4000. The temperature range of the measurements was 80 K – 300 K and a measurement frequency range f=0.2 – 100 Hz. We found distinct temperature and frequency dependences of Young´s modulus of the porous materials filled with water [1], which is explained in terms of a glass to liquid transition depending also on the pore size. Further analysis of the data confirmed that the pore size dependence of T_g is an interfacial rather than a finite-size effect. Extrapolating the relaxation times obtained for water in different confinements to 100 s yields a perfect (1/d)-dependence of $T_g(d)$, which for $d \rightarrow \infty$ yields the traditional glass transition temperature (T_g=136 K) of bulk water [2].
Recent results show that the behaviour of water in the pores at low temperature depends very strongly on the cooling rate (Fig.1).

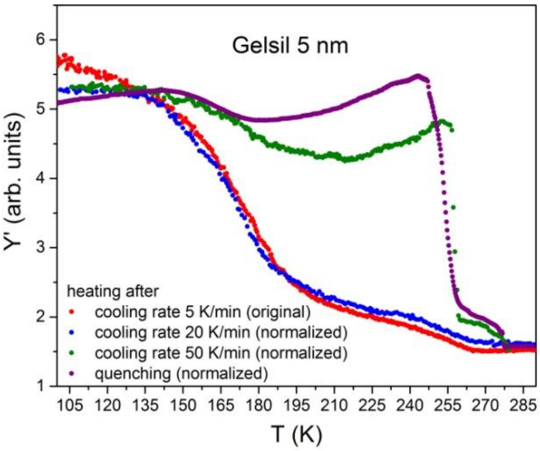

Fig. 1. Comparison of the temperature dependences of Young's modulus of Gelsil (5 nm) filled with water at heating after different cooling rate.

Acknowledgements: The present work was supported by the Austrian Science Fund (FWF, project Nr. P 28672 – N36).

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Poster no. 28

Electric current relaxation processes in non-homogeneous bismuth manganite - lead titanate ceramics induced by annealing in gaseous nitrogen

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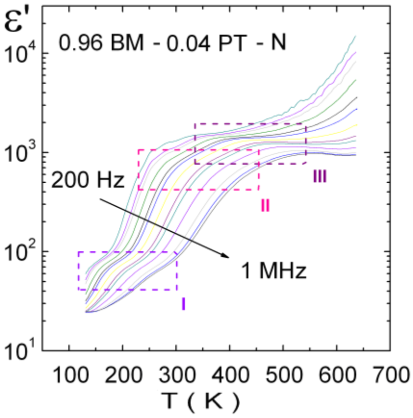
The 0.96Bi-Mn-O–0.04PbTiO$_3$ ceramics was sintered from non-polar bismuth manganite (BM) and ferroelectric lead titanate (PTO) components, at 1170 K and ambient air pressure. The BM-PTO ceramics was annealed in nitrogen N$_2$ flow at 1120 K. The X-ray pattern analysis shown that the ceramics consists of three phases: orthorhombic *Pbmn*, sillenite cubic *I23*, and tetragonal *P4mm.*Scanning electron microanalysis exhibited irregular polyhedron-type shapes of the ceramics grain and non-homogeneous chemical composition. The precipitation of Pb ions and non-uniform distribution of Ti ions related to anti-correlation in distribution of Bi and Mn ions was detected using TOF-SIMS test. The electric impedance was measured in frequency f = 20 Hz – 1 MHz and T = 150–650 K ranges. The BM-PTO ceramics showed two electric conductivity relaxations. Third relaxation processes occurred in the samples annealed in gaseous nitrogen. The characteristic times, $\tau_{0,i}$, were of the order of picoseconds and the activation energy values varied from 0.17 to 0.6 eV. The electric resistivity temperature dependence, with activation energy varied in 0.17-0.46 eV range. The electric features were attributed to the of small polaron hopping model.



Poster no. 29

Magnetostructural correlations in copper cubanes

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The tetradendate Shiff base ligand has been completed with copper(II) giving rise to a a tetranuclear copper(II) complex [Cu_4(3-MeOSAIB)$_4$].H_2O with cubane structure classified according to the number of Cu···Cu contacts and brinding angles Cu-O-Cu, as 4 + 2 cubane. The distances of the cube edges can be distinquished into two types: eight short ones ranging from 1.924 Å to 2.006 Å occuring as the bonds in basal planes, and other four longer ones being of value 2.279 Å by apical coordination (CCDC 916294) [1]. The temperature and field dependence of the magnetic moment of cubane, taken using a SQUID apparatus (MPMS-XL7, Quantum Desing) applying field of B = 0.1 T, exhibit the room-temperature value $(\mu_{\mathrm{eff}})_{300\mathrm{K}}$ = 3.16 μ_B as compared to four uncoupled spins s = ½, i.e $(\mu_{\mathrm{eff}})_{\mathrm{HT}}$ = g[4s(s+1)]1/2 = 3.46 μ_B when g = 2. On cooling the effective magnetic moment decreases progressively that confirms sizable exchange coupling of an antiferromagnetic nature (**Fig. 2**).The magnetic data was fitted by using the spin Hamiltonian that accounts for the isotropic exchange of four Cu(II) centers: $\hat{H} = \mu_B B^A \Sigma_4 g \hat{S}_{az} \hbar^{-1} - J_2[(S_{Cu1}.S_{Cu1'}) + (S_{Cu2}.S_{Cu2'})]\hbar^{-1} - J_4[(S_{Cu1}.S_{Cu2}) + (S_{Cu1}.S_{Cu2'}) + (S_{Cu1'}.S_{Cu2}) + (S_{Cu1'}.S_{Cu2'})]\hbar^{-2}$. The X-ray structure showed that there are two distinct crystallographic centers Cu1 and Cu2 with distances Cu1–Cu1 = 3.427 and Cu2–Cu2 = 3.471 Å, J_2 = J(Cu1–Cu1) = J(Cu2–Cu2), whereas the four remaining contacts are Cu1–Cu2 = 3.333, 3.316, 3.333, 3.316 Å, J_4. The fitting procedure converged to the following set of magnetic parameters: J_2/hc = +6.24, J_4/hc = -80.5 cm^{-1}, g = 2.053, χ_{TIM} = -1.8 10^{-9} m^3 mol^{-1}, χ_{PI} = 0.012. The quality of the fit is perfect as is displayed in Fig. 1; the discrepancy factor R = 0.021. The reported solution of the fitting procedure is stable (the error functional does not change upon variation of J_2). The magnetic structural data of selected complexes with the cubane-type {Cu_4O_4} core, the CCDC offers 131 hits, however, the sources of reliable magnetic data is much less numerous (12 cubanes including [Cu_4(3-MeOSAIB)$_4$].H_2O up to this date).

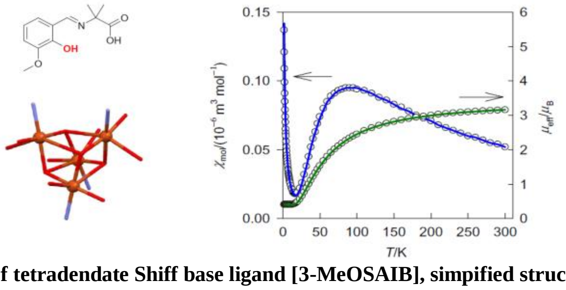

Fig. 1. The structure of tetradendate Shiff base ligand [3-MeOSAIB], simpified structure of Cu(II) cubane [Cu_4(3-MeOSAIB)$_4$].H_2O and the temperature dependence of effective magnetic moment.

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Poster no. 30

Dynamic stimulation of phase transition in Triglycine Sulphate single crystals

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Investigation of pyroelectric properties of triglycine sulfate (TGS) samples using fast temperature pulses in both ferroelectric and paraelectric phases is presented in the paper. Previous experiments proved some kind of order in the paraelectric phase which resulted in electric response to the fast temperature pulses above the critical temperature [1]. Phase transition and structural changes of TGS is being investigated by many authors [2,3]. The aim of this investigations is to find the structural origin of ferroelectricity and explain the mechanism of the phase transition. In our works we use self constructed software and hardware solutions. Results of experiments seem to confirm observations of the evolution of local order despite of order/disorder character of the phase transition in TGS.

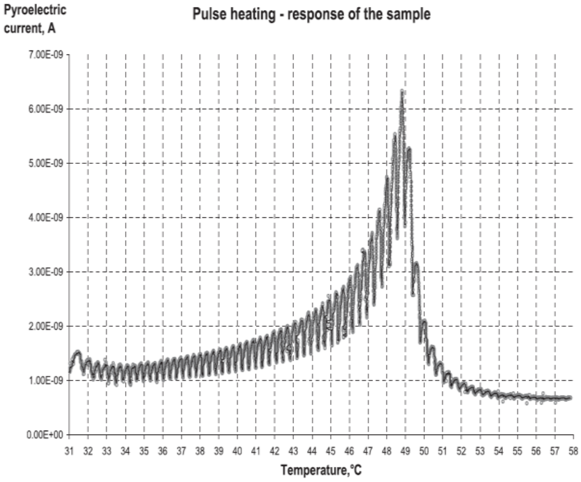

Fig. 1. Pyroelectric response of TGS sample on pulse temperature waveform (B)

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Poster no. 31

The crystal structure of zirconium dioxide partially substituted by Ce ions

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Zirconia composites are materials with unique physical properties: high fracture toughness and a bulk modulus, a high melting point and a low thermal conductivity, chemically inertness and high dielectric constant and etc. Therefore zirconia ceramic has a wide range of application in atomic industry, in biomedical field (dentistry and prosthetics) and etc. In order to control functional properties in microcrystalline zirconia, the stabilization of the tetragonal zirconia phase at room temperature is done by doping it with a large ion such as Y, Ce, Mg, or Ca [1]. The crystal structure of zirconia doped with divalent or trivalent cations contain a deficient in oxygen that favors oxygen transportation and produces ionic conduction. As result, these materials can be used as an oxygen sensor [2] and in the fabrication of fuel cells [3]. The main aim of our work is investigation the influence of Ce ions to phase composition and crystal structure of partially substituted zirconium dioxide and definition the influence on their mechanical properties. The Ce doped zirconia samples ($Zr_{1-x}Ce_xO_2$ ($x = 0–0.17$)) have been obtained through the standard ceramic technology and annealed at 1500^{0}C (6 h). The main feature of our work was application of neutron method with a very high resolution ($\Delta d/d \sim 0.001$) that allowed us to receive the information about microstructure of ceramic samples. The increase of Ce concentration leads to decrease of microstresses in crystaline. Comparison of X-ray and neutron data allowed determining a difference of the phase composition between the surface layer of the sample and the phase composition of the bulk samples.

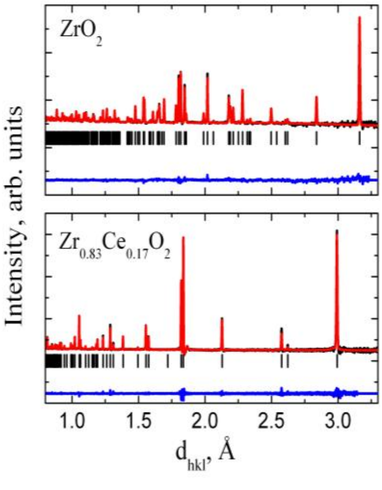

Fig.1. ND patterns of zirconium dioxide partially substituted by Ce ions

[1] E. C. Subbarao, H. S. Maiti, and K. K. Srivastava, Phys. Status Solidi V.21, P.9 (1974).
[2] J.V. Spirig, R.Ramamoorthy, S.A. Akbar et al. Sensors and Actuators, B 124, P.192 (2007).
[3] Albert Tarancyn, Energies, V.2, P.1130 (2009).

Poster no. 32

Temperature dependence of the EMR spectra for $Ni_{50-x}Co_xMn_{35.5}In_{14.5}$ Heusler alloys obtained by melt-spinning process

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Ni-Mn-In and Ni-Co-Mn-In belong to metamagnetic Ni-Co-Mn-X (X = In, Sn, Sb) Heusler alloys family and shown many promising physical properties, e.g. giant invers magnetocaloric effect, which can be applied in ecological refrigeration. Some properties of these materials, e.g. temperature of martensite transition, could be tuned by appropriate choice of chemical composition of the alloy. One of the problems with application of Ni-Mn-In in industry is its brittleness. The addition of Co reduces brittleness and improves plasticity. Additionally, an increase of Co content up to 5 % at. changes temperature of matrensite transition and shift Curie temperature into the higher region.

In this research we registered electron magnetic resonance (EMR) spectra of off-stoichiometric $Ni_{50}Mn_{35.5}In_{14.5}$ and $Ni_{45}Co_5Mn_{35.5}In_{14.5}$ ribbons which were obtained by melt-spinning process. Temperature dependences of the EMR spectra was recorded in the temperature range 180-300 K.

[1] R. Kainuma et al., J. Mater. Chem. **18** (2008) 1837.
[2] T. Kanomata et al., Magn. Magn. Mater. **321** (2009) 773–776.
[3] W. Ito et al., Metall. Mater. Trans. A Phys. Metall. Mater. Sci. **38** (2007) 759–766.
[4] W. Maziarz, Solid State Phenom. **186** (2012) 251–254.

Poster no. 33

Structural and dielectric characterization of haloantimonates(III) and halobismuthates(III) based on diisopropylammonium cations

M. Wojciechowska[1], A. Białońska[1], A. Piecha-Bisiorek[1], R. Jakubas[1]

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The field of ferroelectricity has greatly expanded and changed recently. In addition to the classical organic and inorganic as well as composite ferroelectrics new fields and materials have appeared, important for both basic science and application and showing technological promise for novel multifunctional devices. [1-2] The most spectacular example of such compounds is diisopropylammonium bromide (DIPAB), characterized by extremely high value of spontaneous polarization (23 $\mu C/cm^2$) comparable to the inorganic oxide ferroelectrics of the perovskite type ($BaTiO_3$). [3] On the other hand, in the group of organic-inorganic hybrid compounds, based on Sb(III) and Bi(III), ferroelectricity is limited only to several chemical compositions, *e.g.* RMX_4, $R_3M_2X_9$, R_2MX_5 and $R_5M_2X_{11}$ (where: where R denotes organic cation, M stands for Sb or Bi and X = Cl/Br/I). [4] As regards the first presented, up to now the ferroelectric properties have been observed only for two different analogs, namely: $[4\text{-}NH_2C_5H_4NH][SbCl_4]$ [4] and $(TAMS)Bi_2Cl_8$ [5] (where $TAMS^{2+}$ = trimethylamino-N-methyl stilbazolium). Taking above into account we have decided to extend our studies and to use diisopropylammonium cation in search for new, polar materials within the group of haloantimonates(III) and halobismuthates(III). We have thus synthesized for diisopropylammonium analogues with the chemical stoichiometry RMX_4. The physicochemical properties of these compounds were characterized by using single crystal X-ray diffraction, dielectric spectroscopy and ^1H NMR spin-lattice relaxation methods.

[1] M. Owczarek, K. A. Hujsak,D. P. Ferris, A. Prokofjevs, I. Majerz, P. Szklarz, H. Zhang, A. A. Sarjeant, C. L. Stern, R. Jakubas, S. Hong, V. P. Dravid, J. F. Stoddart, Nat. Commun. **7**, 13108 (2016)
[2] J. F. Scott, Science **315**, 954 (2007)
[3] A. Piecha, A. Gągor, R. Jakubas, P. Szklarz, CrystEngComm 15, 940 (2013)
[4] L. Sobczyk, R. Jakubas, J. Zaleski, Pol. J. Chem. **71**, 265 (1997)
[5] R. Jakubas, Z. Ciunik, G. Bator, Phys. Rev. B **67**, 1 (2003).

This research project was financed by the KNOW grant no 12 (R. Jakubas)

Poster no. 34

Electron energy spectrum in 2D quantum dot

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Semiconductor quantum dots introduced into photoelectric materials are currently very important and effective way to increase the efficiency of photoelectric devices and photovoltaic cells. This is related to the appearance of additional energy levels in the system, and it expands the range of absorption frequencies toward the infrared.

This work contains the theory and numerical calculation of energy levels in quantum dots in perovskite solids. The model of the structure includes a semiconductor quantum dot shaped in nanodisk which is surrounded by another semiconductor. The calculations of the energy levels as functions of the dot radius and various types of semiconductors materials are performed. We also discuss the creation of energy bands related to the electron hopping between the quantum dots.

Poster no. 35

Multiferroic Hübnerite with unusual high molybdenum doping studied by x-ray powder diffraction and Raman spectroscopy

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The physical properties of Hübnerite ($MnWO_4$) have been widely investigated over the last years since this material serves as model substance for type II multiferroics with spiral spin order. While their coupling of magnetic and electric properties seems promising for future applications, they all suffer from impractical low phase transition temperatures. Recently, it was shown for $MnWO_4$ that these temperatures can be increased when tungsten atoms are substituted by molybdenum [1,2]. The published maximum doping concentration varies in the range of $0.1 \leq x \leq 0.3$. Therefore, the aim of the present investigation is to increase the molybdenum content in the wolframite phase as high as possible using different synthesis strategies and avoiding the formation of a molybdate phase.

We prepared powder samples with a variety of different molybdenum contents in the range of $0 \leq x \leq 1$. All samples were produced by solid state reaction with a variation of the reaction temperature and characterized by x-ray powder diffraction and Raman spectroscopy. With a careful synthesis from the pure metal oxides at low temperatures it is possible to suppress the formation of the molybdate phase and reach higher doping concentrations than previously published. Indeed, it is possible to prepare a sample with nearly 70% molybdenum in the wolframite phase as reflected by the x-ray pattern (see Fig. 1) as well as by characteristic stretching vibrations in the Raman spectra. An increase of the phase transition temperatures was verified by measuring the magnetic susceptibility.

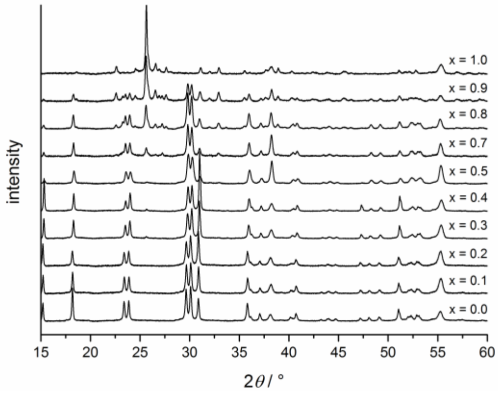

Fig. 1. : X-ray powder diffraction pattern for different amounts of molybdenum.

[1] L. Meddar et al., Chem. Mater., 2012, 24, 353−360.
[2] L. L. Y. Chang, Mineral. Mag., 1968, 36, 992-996.

Poster no. 36

New composite gyrotropic metamaterial

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This work is the continuation of our study started in Ref. 1. In it, we examined the possibility of fabricating the metamaterial in a relatively simple way. Our idea was to use the three-component mixture of ingredients, where one of them is responsible for the negative permeability $\mu(\omega)$ of hypothetical metamaterial while the other two cause the negative value of effective permittivity $\varepsilon(\omega)$. In our previous work, we considered $Hg_{1-x}Cd_xTe$ semiconductor compound as one of the ingredients of the mixture. As fabrication of the $Hg_{1-x}Cd_xTe$ is related to using mercury which is very poisoning, we tried to exclude this material. In the work, we proved by numerical simulations the possibility of substituting mercury cadmium telluride by $Pb_{1-x}Sn_xTe$. We have shown by computer simulations that by the proper fitting of the parameters, e.g. the radius of nanoparticles, their magnetic moments, the relative concentration of ingredients etc., it is possible to obtain the metamaterial with negative refraction index in a relatively broad range of temperatures and magnetic fields. The last seems to be very promising in terms of practical applications of metamaterials.

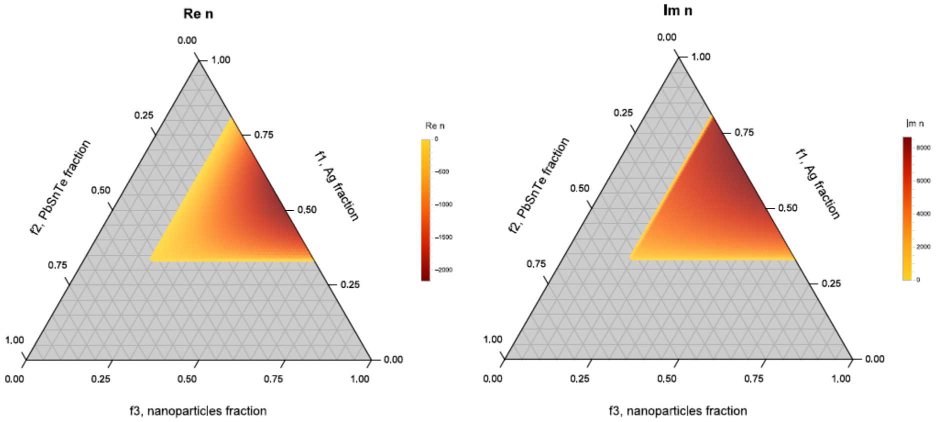

Fig. 1. Real and imaginary parts of the refractive index of the composite for selected cases presented on the ternary diagram. On each axis of the triangle the relative contribution of individual components of the composite are indicated, which are expressed as the values of the filling factors f1, f2, f3. Model parameters: $B = 0.4T$, $r = 8nm$, $m = 103\mu_B$, $T = 290K$, $x = 0.08$.

[1] I.Tralle, P. Zieba and W. Pasko, *J. Appl. Phys.* **115**, 233509 (2014).

Poster no. 37

Zitterbewegung and symmetry switching in the Klein's four-group

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Zitterbewegung is the exotic phenomenon associated either with the relativistic electron-positron rapid oscillations, or to the electron-hole transitions in the narrow gap semiconductors [1,2]. In the present work we enlarge concept of Zitterbewegung and show that trembling motion may occur due to the dramatic changes in the symmetry of the system. In particular, we exploit paradigmatic model of quantum chaos, quantum mathematical pendulum (universal Hamiltonian). Symmetry group of this system is the Klein's four-group that posses three invariant subgroups. Energy spectrum of the system parametrically depends on the height of the potential barrier, and contains degenerate and non-degenerate areas, corresponding to the different symmetry subgroups. Change in the height of the potential barrier switches the symmetry subgroup and leads to the trembling motion. We analyzed the mean square fluctuations of the velocity operator and observed that trembling enhances for the high exited states.

[1] E. Schroedinger, *Sitzungsb. Preuss. Akad. Wiss. Phys. Math. Kl.* **24**, 418 (1930).
[2] W. Zawadzki, T.M. Rusin, *J. Phys. Condens. Matter* **23** 143201 (2011).

Video lecture to be presented during poster sessions

Choreographic crystals

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[1]*Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada*
[2]*MIT Physics Department, Cambridge, MA 02139, USA*
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I will introduce a natural dynamical analogue of crystalline order, which I call choreographic order [1,2]. I will illustrate the idea with some interesting examples of choreographic crystals. I will explain how to classify such systems mathematically, and how to identify the most "highly choreographed" cases. Finally, I will discuss some thoughts about how to create or detect choreographic crystals in the lab.

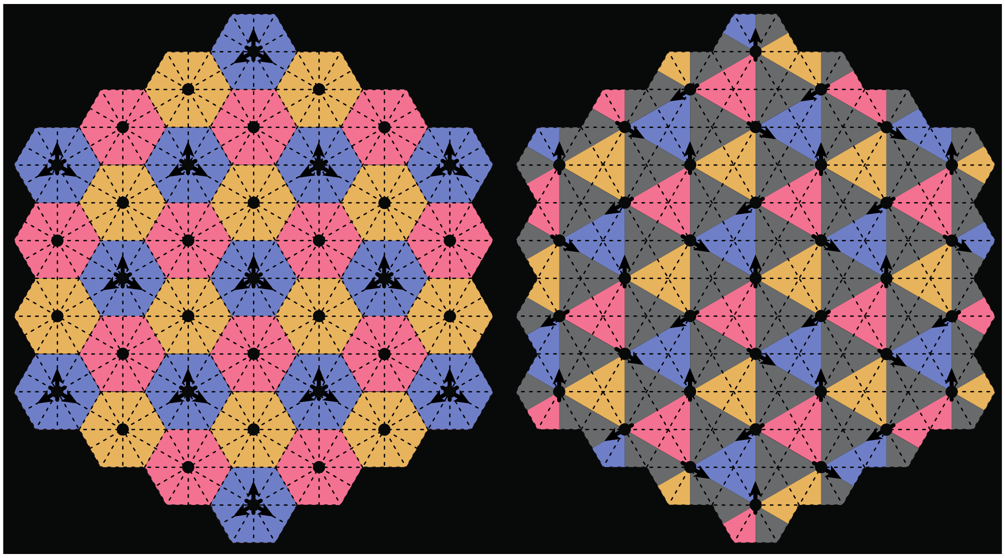


Fig. 1. Snapshots of (hexagonal pieces of) two planar choreographic crystals.

The original reference is [1]. For a non-technical introduction, see [2].

[1] L. Boyle, J.Y. Khoo, K. Smith, Phys. Rev. Lett. **166**, 015503 (2016).
[2] L. Grossman, "Physicists dream up crystal based on elegant satellite dance," Jan 23 2016 issue of New Scientist (also available online).

Events and Venues

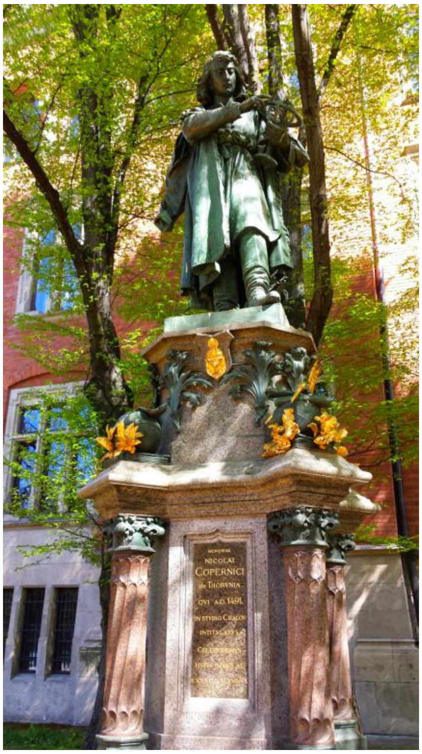
Opening session in honour of Marian Smoluchowski

The opening session will take place in Collegium Witkowski of the Jagiellonian University, 13 Gołębia Street (Dove Street). The building was erected in years 1908 – 11. The initiator of the construction, August Witkowski, was professor of physics and Rector Magnificus of the University. The building housed the Physics Department till 1964, the 600-th anniversary of the University.

Marian Smoluchowski (born on 28 May 1872 in Vorder-Brühl near Vienna, – died on 5 September 1917 in Kraków), was the successor of August Witkowski, moved to Kraków from Lwów (Ukr. Lviv) to take over the chair in the Experimental Physics Department in 1913. When World War I began, the work conditions became difficult, since the building was converted into a military hospital.

The opening lecture is to be given by Prof. Józef Spałek from the Institute of Physics of Jagiellonian University. He is a physicist and renowned university lecturer. He received the Prize of the Foundation for Polish Science in 2016, in the mathematical, physical, and engineering sciences for his research on strongly correlated electron systems and in particular, for the derivation of the so-called t-J model.

The opening ceremony will be accompanied by a concert of the choir Cantata of Cracow University of Technology, conducted by Marta Stós.

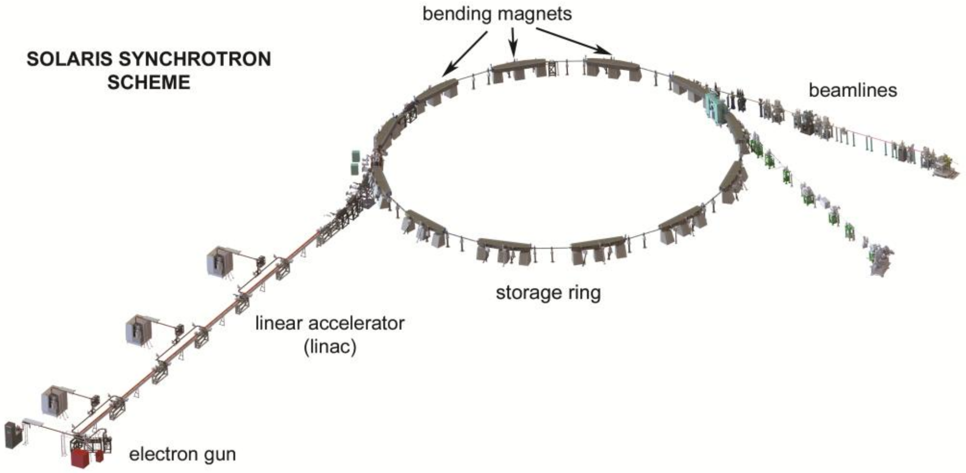


Monument of Nicolaus Copernicus, student of Cracow Academy (today Jagiellonian University) in 1491-1495, in front of Collegium Witkowski

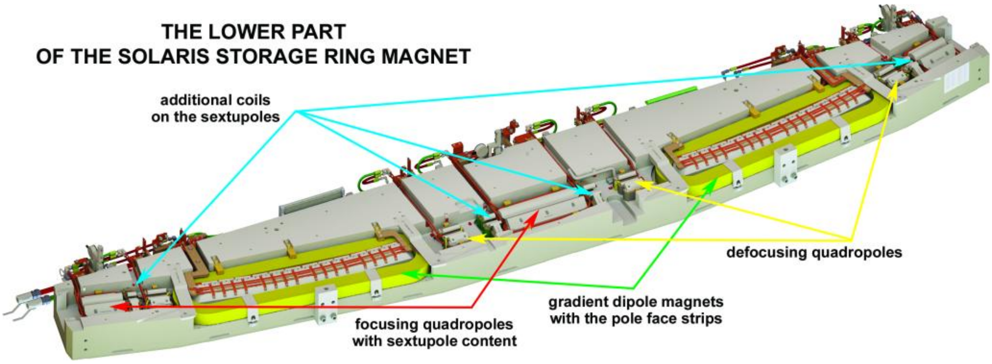
Collegium Witkowski, façade

Solaris Synchrotron

SOLARIS is a brand new “fourth generation” synchrotron radiation source located in Kraków, Poland. The National Synchrotron Radiation Centre SOLARIS was built between 2010 and 2015. The synchrotron itself was launched in September 2015. Since then a team of over 40 people has been working to make the infrastructure available for scientists: to achieve optimum synchrotron parameters and to start operation of two beamlines: the PEEM/XAS beamline for a photoemission electron microscopy/X-ray absorption spectroscopy, and the UARPES beamline for an ultra-angle resolved photoemission spectroscopy.



The commissioning of the beamlines started right after the synchrotron had been launched. In June 2016 the UARPES team did, for the first time, a typical experiment for which the beamline had been designed – the massively parallel angle-resolved photoelectron spectroscopy mode were tested. In the same time in the SOLARIS storage ring more than 400 mA of beam current was ramped to the final 1,5 GeV energy. In May 2017 first photons reached PEEM/XAS beamline components. The end of beamlines commissioning is planned for the beginning of the next year.



In 2016 and 2017 the SOLARIS Centre acquired funds for the construction of two more beamlines: the PHELIX beamline for a photoelectron spectroscopy and the XMCD beamline for a X-ray magnetic circular dichroism.

Sessions: Palace Łobzów

The lecture hall and the poster exposition room of DyProSo2017 are located in the former Royal Palace Łobzów, 1 Podchorążych Street (Cadet Street), that houses nowadays two faculties of The Cracow University of Technology: Faculty of Architecture, and Faculty of Physics, Mathematics and Computer Science. The beginnings of the edifice go back to the times of King Casimir the Great who built here, in 1357, a small castle, may be for his half-legendary mistress Esterka (Esther). About hundred years later the chronicler Jan Długosz noted: “(...) the Polish king Kazimierz (...) took as his concubine a woman Esther of Jewish descent, because of her extraordinary beauty. ... At the request of Esther, the royal document also granted to all Jews living in the Kingdom of Poland extraordinary privileges and freedoms.” Reportedly, the king had casted up a mound after Esterka’s death. The mound still existed in the fifties of the 20th century in the park surrounding the palace. As a result of a reconstruction started by King Sigismund the Old in 1522 and accomplished by King Stefan Batory in 1585-1587, a mannerist palace with arcades replaced the initial gothic fortress.

Bust of Marshal Józef Piłsudski (1867 – 1935) in front of former royal palace Łobzów

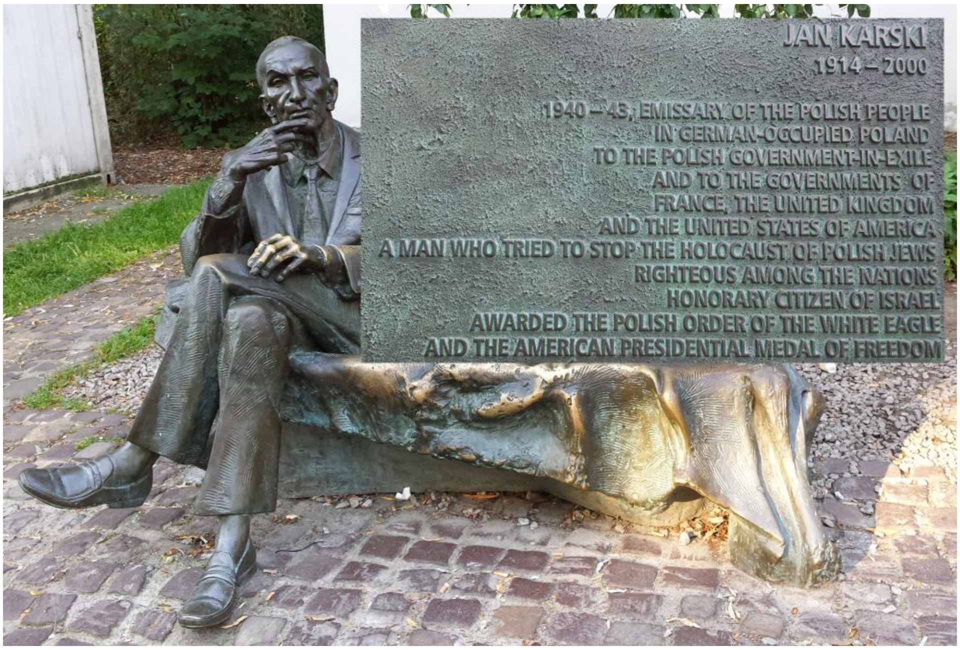
The palace became a frequent royal residence under the reign of Sigismund III Vasa who, on the other hand, had moved Poland’s capital to Warsaw. In the ground floor corridor we will find a portrait of the King Władysław IV Vasa born in this building. Restored after the Swedish “deluge” (1655) the palace witnessed to the triumphal return of King Jan III Sobieski from the victorious relief battle of Vienna (1683). War trophies were also displayed here. Under the Austrian rule in the partition times (1795 – 1918), the palace was transformed into a Cadet Institute of Artillery (1852) with substantial reconstructions lead by Feliks Księżarski, the architect of the Collegium Novum of the Jagiellonian University. Evoking remains of this military function of the building can be seen in the main staircase. After World War II numerous former Austrian caserns have been given to the newly organized school of engineers, initially Polytechnic Faculties within the Academy of Mining and then, since 1954, the independent Cracow University of Technology. The staff of the new university included mainly Polish researchers and teachers expatriated from the leading academic centre Lwów (Ukr. Lviv). Prof. Tadeusz Malarski from the Lwów Polytechnic founded the Chair of Physics. His successor, prof. Michał Halaubrenner, an alumnus of the Jan Kazimierz University of Lwów and teacher at the Casimir the Great High School in Lwów was an author of numerous textbooks on physics for various grades of education. The Chair, later transformed into the Institute of Physics of the Cracow University of Technology, has found its seat in the Palace Łobzów. Careful restoration works still aim at preserving as many as possible historical details, e.g. the ceiling in the lecture room W1. Now the surrounding park is progressively regaining its splendor and the Esterka's mound will hopefully also come back to its place soon.

Conference dinner: District Kazimierz

The conference dinner will take place in the restaurant Szara Kazimierz, 39 Szeroka Street (Eng. Broad Street), located in the district Kazimierz of Kraków. The quarter bears its name after the king Casimir III the Great (Kazimierz III Wielki) who founded here, on an isle on the Vistula River, a new town Casimiria in 1335 and fortified it soon after. The king, remembered as the one who "found a Poland made of wood and left it made of stone", founded in 1364 the first Polish university (Studium Generale, today Jagiellonian University) with its first campus in Kazimierz. The king also extended over his whole country the privileges granted to Jews in 1264 in the Great Poland. The years of pest, 1347 – 1351, marked an intense influx of Jews who were elsewhere blamed for the plagues and persecuted. The Jewish population of Cracow was settled in a part of Kazimierz (Bawół – Bufallo) in 1495 by the king Jan I Olbracht. The town, oppidum iudaeorum, became an important centre of Jewish culture in Poland. A famous Rabbi Moses ben Israel Isserles, abbr. Remu, (ca. 1525, Kazimierz – 1572, Kazimierz) wrote to one of his pupils: "Had not the Lord left us this land as a refuge, the fate of Israel would have been really unbearable." The building next to the restaurant Szara is just the synagogue Remuh, built by Israel ben Josef, the father of the Rabbi, in honour of his son in the years 1553 – 1557. The Remu's tombstone at the neighbouring Remuh Cemetery survived miraculously the occupation of 1939-1945 and still attracts pilgrims from all over the world. The Kazimierz's oldest synagogue, called Old Synagogue, started probably in 1407, is situated at the end of the Szeroka Street. The town was formally incorporated into the great Kraków at the end of the 18th century. The walls of the Jewish part were demolished in 1822 and the separating branch of the Vistula River was filled and transformed into an important artery (Józef Dietl Street) in 1878 -1880. However, the living conditions in Kazimierz degraded with time. The life of Leopold Infeld (1898 – 1968), a son of a leather merchant from Kazimierz and later a co-worker of A. Einstein, W. Heisenberg and M. Born, is an example of difficulties in getting out of the poverty and ethnic isolation. In March 1941 the German Nazi expelled the Jewish population of Kazimierz to the ghetto located in the district Podgórze on the other side of the Vistula River. The ghetto was liquidated between June 1942 and March 1943. Most of its inhabitants were sent to the concentration camps at Bełżec, Oświęcim (Auschwitz) and Płaszów. The latter, also situated in the district Podgórze, is particularly known from the Oskar Schindler's factory described in the novel "Schindler's Ark" by Thomas Keneally filmed by Steven Spielberg (1993). With the advent of the transformations of 1989 the district of Kazimierz, so far abandoned and neglected, has been systematically restored in major part by Jewish organizations and private investors. A growing Jewish Culture Festival is organized here every year http://www.jewishfestival.pl/en/jewish-culture-festival/. Some streets in the quarter Kazimierz bear the names of heroes of the Old

Testament: Isaac, Jacob, Joseph, Ester. The Lewkowa Street commemorates Lewko (? - 1395), a rich royal banker and tenant of the salt mines. Dr. Jonatan Warszauer (1820 -1888) was a physician who worked for the poorest inhabitants of Kraków and Kazimierz. Rabbi Dow Ber Meisels (1798 –1870) and colonel Berek Joselewicz (1764 – 1809) contributed to the Polish struggle for independence.

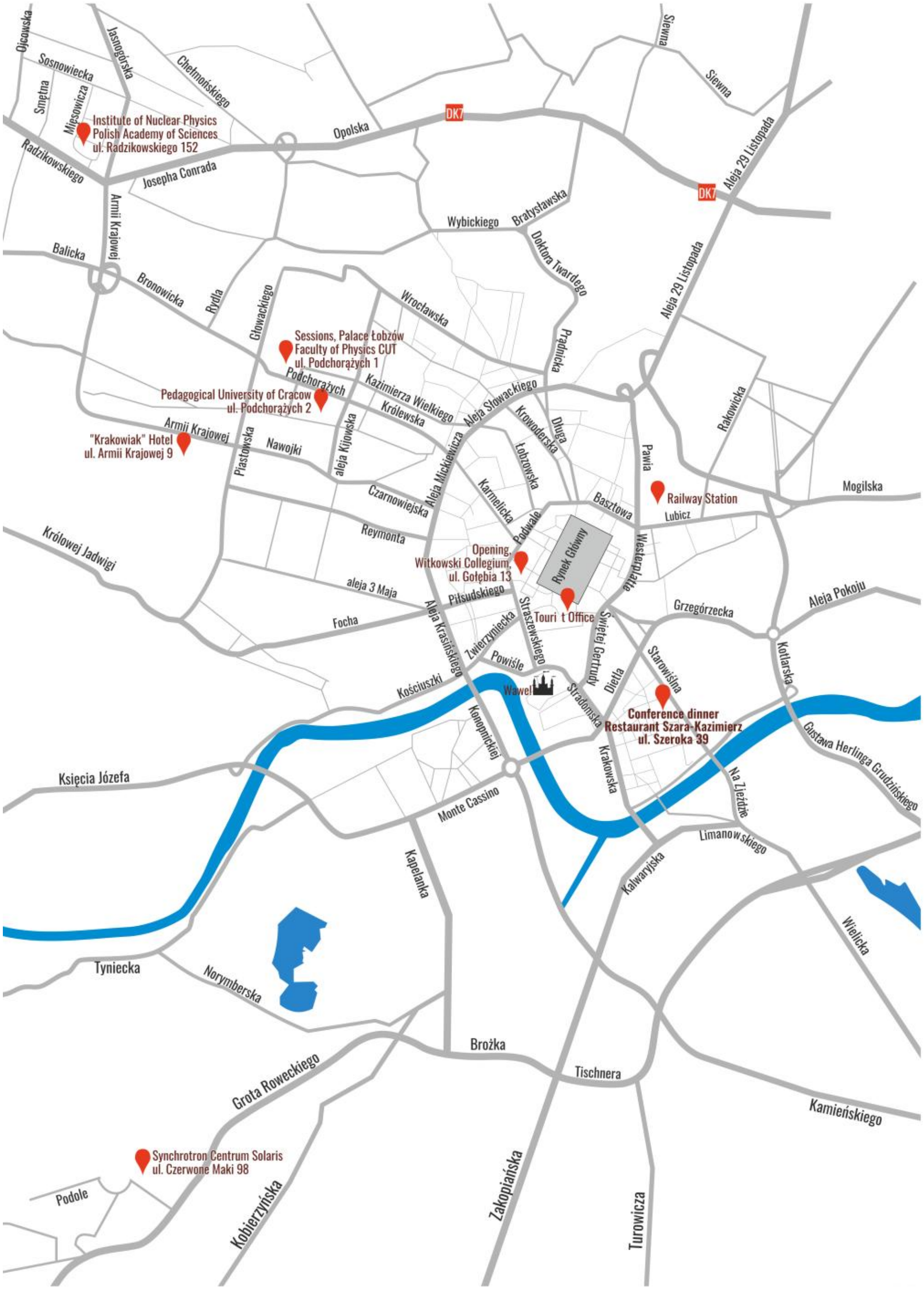
Restaurant Szara Kazimierz, 39 Szeroka Street, and entrance to the Remuh Synagogue



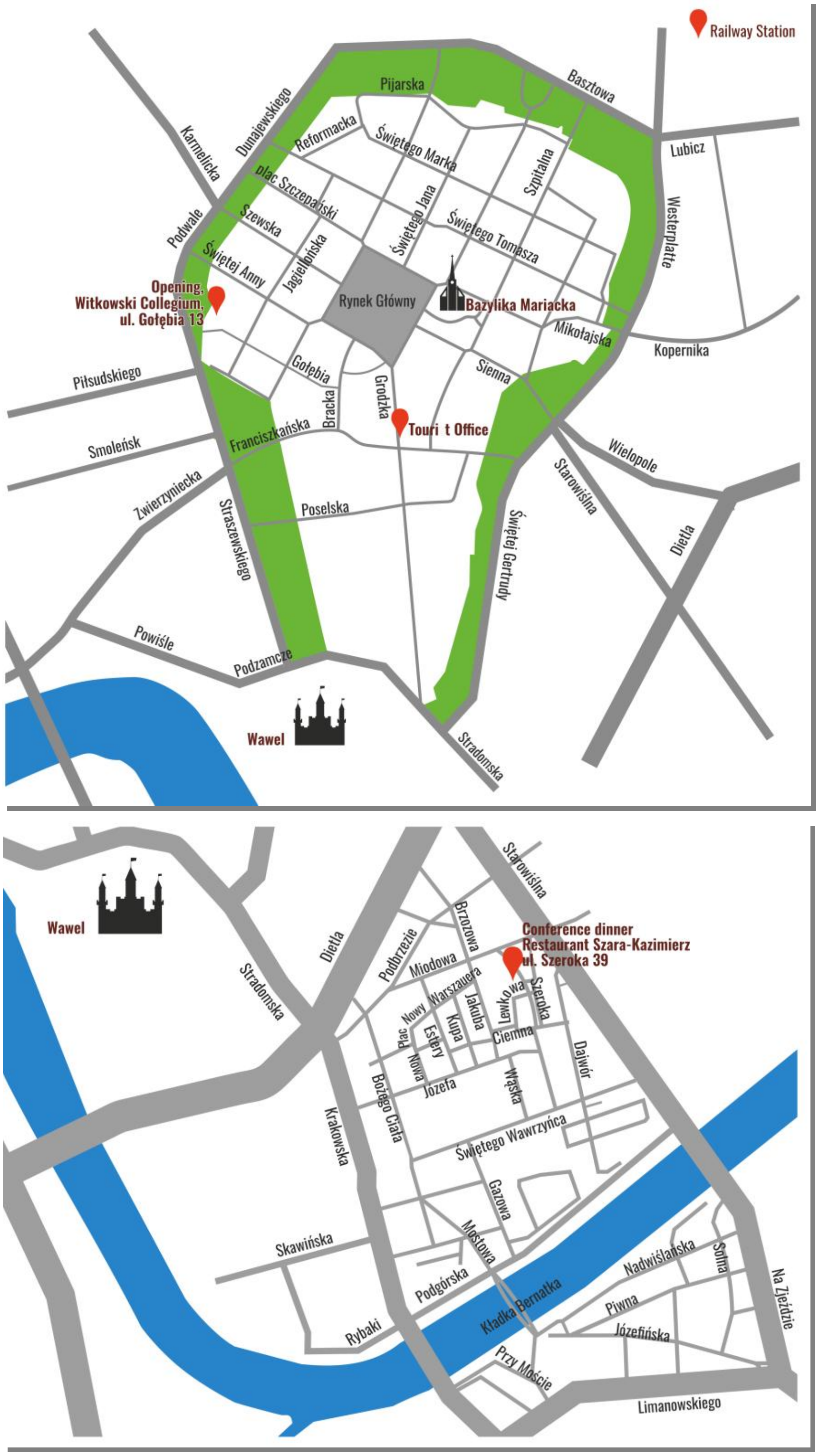
Jan Karski bench next to Remuh Synagoue

Author: Piotr Zieliński

City map: locations important for DyProSo 2017



City map: locations important for DyProSo 2017



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Sunday 27 VIII – The Collegium Witkowski, Jagiellonian University, 13 Gołębia Street

Time	Event
13:00–17:00	Registration
17:00–17:20	Opening Ceremony
17:20–18:05	Opening Lecture Józef Spałek "Many particle physics: From Smoluchowski to the quantum strongly correlated matter"
18:05–20:30	Welcome Party

Monday 28 VIII, Tuesday 29 VIII, Wednesday 30 VIII, Thursday 31 VIII – Palace Łobzów, Faculty of Physics, Cracow University of Technology, 1 Podchorążych Street

Monday 28 VIII

Time	Event	Section
08:00–09:00	Registration	
09:00–09:25	Björn Wehinger	VI
09:25–09:50	Andreas Tröster	VI
09:50–10:05	Matthew Krzystyniak	VI
10:05–10:20	Jiří Hlinka	VI
10:20–10:35	Ivan Gregora	VI
10:35–10:45	Matthias Gutmann	VI
10:45–11:15	Coffee Break	
11:15–11:40	Catalin Gainaru	V
11:40–11:55	Andrzej Budziak	V
11:55–12:10	Vasily Artemov	V
12:10–12:20	Robert Gębarowski	V
12:20–12:35	Zbigniew Łodziana	V
12:35–12:50	Aristea Maniadaki	V
12:50–13:05	Andrzej Molak	V
13:05–14:00	Lunch Break	
14:00–14:10	Izabela Biało	X
14:10–14:20	Łukasz Dubiel	X
14:20–14:30	Fabio Figueiras	X
14:30–14:40	Peio Garcia Goiricelaya	X
14:40–14:50	Katharina Holzweber	X
14:50–15:00	Grzegorz Jagło	X
15:00–15:10	Jochen Kalt	X
15:10–15:20	Magdalena Krupska	X
15:20–15:30	Rafał Kuna	X
15:30–15:50	Marek Stankiewicz (Synchrotron Solaris)	
15:50–16:25	Coffee Break	
16:25–16:50	Alexei Sokolov	I
16:50–17:05	Małgorzata Jasiurkowska-Delaporte	I
17:05–17:20	Natalia Osiecka	I
17:20–17:35	Ewa Juszyńska-Gałązka	I
17:35–17:50	Andriy Kityk	I
17:50–18:05	Paweł Karbowniczek	I
18:05–19:20	Poster Session	XI

Tuesday 29 VIII

Time	Event	Section
08:00–09:00	Registration	
09:00–09:25	Annette Bußmann-Holder	II
09:25–09:40	Jarosław Jędryka	II
09:40–09:50	Gabriela Lewińska	II
09:50–10:00	Grigory Arzumanyan	II
10:00–10:15	Joaquim Agostinho Moreira	VII
10:15–10:25	Paweł Śliż	VII
10:25–10:35	Andrzej Wal	VII
10:35–10:50	Urszula Wdowik	VII
10:50–11:15	Coffee Break	
11:15–11:40	Marek Paściak	III
11:40–11:55	Jan Petzelt	III
11:55–12:10	Stanislav Kamba	III
12:10–12:20	Martin Kempa	III
12:20–12:35	Grażyna Bator	III
12:35–12:45	Renata Bujakiewicz-Korońska	III
12:45–14:00	Lunch Break	
14:00–14:10	Dominika Kuźma	X
14:10–14:20	Jon Lafuente-Bartolome	X
14:20–14:30	Marcin Majka	X
14:30–14:40	Karolina Martinson	X
14:40–14:50	Maria Podgórna	X
14:50–15:00	Sabine Puchberger	X
15:00–15:10	Tomasz Skóra	X
15:10–15:20	Anna Szeremeta	X
15:20–15:30	Daria Szewczyk	X
15:30–15:40	Anton Tuluk	X
15:40–15:50	Rui Vilarinho	X
15:50–16:25	Coffee Break	
16:25–16:50	Stéphane Rols	VIII
16:50–17:05	Zoryana Usatenko	VIII
17:05–17:15	Natalia Nosidlak	VIII
17:15–17:30	Marek Przybylski	VIII
17:30–19:00	Poster Session	XI
19:00–19:30	Meeting of International Advisory Board	

Wednesday 30 VIII

Time	Event	Section
08:00–09:00	Registration	
09:00–09:25	Svetoslav Stankov	VI
09:25–09:40	Radosław Strzałka	VI
09:40–09:55	Wojciech Szuszkiewicz	VI
09:55–10:10	Kamil Tokar	VI
10:10–10:25	Paweł Jochym	VI
10:25–10:50	Krzysztof Parliński	VI
10:50–11:15	Coffee Break	
11:15–11:30	Dominik Legut	VI
11:30–11:40	Paweł Sobieszczyk	VI
11:40–12:05	Zach Evenson	I
12:05–12:20	Agnieszka Chrzanowska	I
12:20–12:35	Łukasz Laskowski	I
12:35–13:35	Lunch Break	
16:30–19:30	Excursion (Starting point: The Collegium Witkowski, 13 Gołębia Street)	
19:30–22:00	Conference Dinner, (Szara Kazimierz Restaurant, 39 Szeroka Street)	

Thursday 31 VIII

Time	Event	Section
08:00–09:00	Registration	
09:00–09:25	Andreas Borgschulte	IX
09:25–09:50	Martin Müeller	IX
09:50–10:00	Adam Szmagliński	IX
10:00–10:25	Vincenzo Guidi	IX
10:25–10:40	Giacomo Gadda	IX
10:40–11:10	Coffee Break	
11:10–11:35	Federico Montoncello	IV
11:35–12:00	Maciej Krawczyk	IV
12:00–12:10	Jarosław Kłos	IV
12:10–12:25	Mirosław Łabuz	IV
12:25–12:40	Zbigniew Tomkowicz	IV
12:40–12:55	Yevhen Zabila	IV
12:55–13:10	Michał Krupiński	IV
13:10–13:25	Conference closing	
13:25–14:25	Lunch Break	

▨	I	Amourphous and soft matter
▨	II	Optoelectronics and magnetooptics
▨	III	Ferroics, multiferroics, ferroelectrics and relaxors
▨	IV	Spins and magnetics systems
▨	V	Diffusive dynamics and relaxations
▨	VI	Lattice vibrations and phonons
▨	VII	Electron extitations
▨	VIII	Low dimentional systems and nanoparticles
▨	IX	Applications and interdisciplinary subject
▨	X	Short communications - competition session
▨	XI	Poster session

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