Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks and Sessions

(lecture rooms H 1, H 3, H 4, H 8, H9, H 11, H 38, and H 48; poster A and D1)

Invited Talks

DF 4.1	Mon	10:15–10:45	H3	**Antiferromagnetic interlayer coupling in $La_{0.7}Sr_{0.3}MnO_3$ / $SrRuO_3$ superlattices** — •Ionela Vrejoiu
DF 6.1	Tue	10:00–10:40	H11	**Gate Oxides beyond SiO_2 and the High K Materials Revolution** — •Darrell Schlom
DF 6.4	Tue	11:35–12:15	H11	**Aspect Ratio Trapping: A Heterointegration Solution for Ge and III-V CMOS** — •James Fiorenza
DF 9.1	Wed	10:00–10:35	H11	**Structural dynamics in photoexcited molecules** — •Majed Chergui
DF 9.5	Wed	11:40–12:15	H11	**Ultrafast photochromism of fulgides** — •Markus Braun, Simone Draxler, Thomas Brust, Stephan Malkmus
DF 10.1	Wed	14:00–14:40	H11	**Molecular self-assembly on calcite** — •Angelika Kühnle, Philipp Rahe, Jens Schütte, Sebastian Rode
DF 14.1	Wed	14:00–14:30	H48	**New Approach to the Old Problem: Cooperativity in Dynamics of Glass Forming Systems** — •Alexei Sokolov
DF 14.6	Wed	15:45–16:15	H48	**Slow domains percolation in polymer melts and blends close to the glass transition: a unifying concept regarding bulk dynamics, dynamics in the vicinity of interfaces, and the physical properties of nanocomposites** — •Didier R. Long
DF 15.1	Thu	10:00–10:40	H11	**Photons meet sound waves** — •Jan K Krüger, Roland Sanctuary
DF 16.1	Thu	14:00–14:40	H11	**Succesive phase transitions in $(Gua)_4SO_4Cl_2$ crystal - dielectric, pyroelectric, dilatometric and optical studies** — •Zbigniew Czapla, Artur Rokosa, Slawomir Dacko, Boguslaw Kosturek

Tutorial: Functional (oxide) single crystals and epitaxial films - from growth to function

DF 1.1	Sun	16:00–16:45	H4	**Influence of ferroelectric phase transitions on the melt growth of bulk oxide crystals** — •Manfred Mühlberg, Manfred Burianek
DF 1.2	Sun	16:45–17:30	H4	**Electromechanical properties of crystals** — •Eiken Haussühl
DF 1.3	Sun	17:30–18:15	H4	**Epitaxial ferroelectric oxide thin films, nanostructures, and superlattices** — •Dietrich Hesse, Ionela Vrejoiu, Marin Alexe

Focus Session: High-k and high mobility materials for CMOS

Organisation: Thomas Schröder und Jürgen Schubert

DF 6.1	Tue	10:00–10:40	H11	**Gate Oxides beyond SiO_2 and the High K Materials Revolution** — •Darrell Schlom
DF 6.2	Tue	10:45–11:10	H11	**Advanced CMOS transistor technologies using HKMG and strained Silicon for high performance applications** — •Manfred Horstmann
DF 6.3	Tue	11:10–11:35	H11	**Amorphous ternary high-k oxides on Si and higher mobility substrates** — •Marcelo Lopes, Eylem Durgun-Ozben, Alexander Nichau, Roman Luptak, Martin Roeckerath, Juergen Schubert, Siegfried Mantl

DF 6.4	Tue	11:35–12:15	H11	**Aspect Ratio Trapping: A Heterointegration Solution for Ge and III-V CMOS** — •James Fiorenza
DF 6.5	Tue	12:20–12:45	H11	**Wafer Bonding Techniques for Advanced CMOS** — •Manfred Reiche
DF 6.6	Tue	12:45–13:10	H11	**Si wafer engineering: single crystalline oxides as buffers for the integration of alternative semiconductors** — •Alessandro Giussani, Peter Zaumseil, Olaf Seifarth, Markus Andreas Schubert, Peter Storck, Thomas Schroeder

Focus Session: Structural dynamics in photoexcited molecules

Organisation: Dominik Schaniel

DF 9.1	Wed	10:00–10:35	H11	**Structural dynamics in photoexcited molecules** — •Majed Chergui
DF 9.2	Wed	10:40–11:00	H11	**Ultrafast reversible photogeneration of nitrosyl linkage isomers in $Na_2[Fe(CN)_5NO]2H_2O$** — •Matthieu Nicoul, Theo Woike, Dominik Schaniel
DF 9.3	Wed	11:00–11:20	H11	**Photoinduced isomerization of molecular switches at metal surfaces** — •Petra Tegeder
DF 9.4	Wed	11:20–11:40	H11	**Light induced conformational changes of retinal proteins** — •Heinz-Jürgen Steinhoff
DF 9.5	Wed	11:40–12:15	H11	**Ultrafast photochromism of fulgides** — •Markus Braun, Simone Draxler, Thomas Brust, Stephan Malkmus
DF 9.6	Wed	12:20–12:40	H11	***Ab-initio* and semi-empirical molecular dynamics studies of photoisomerisable molecules** — •Jan Boyke Schönborn, Ole Carstensen, Bernd Hartke
DF 9.7	Wed	12:40–13:00	H11	**Influence of ligand substitution and dielectric environment on structural dynamics in photoswitchable molecular compounds** — •Volker Dieckmann, Sebastian Eicke, Kristin Springfeld, Mirco Imlau

Symposium Density Functional Theory and Beyond for Real Materials (SYDF)

See SYDF for the full program of the sympsium

SYDF 1.1	Thu	14:45–15:15	H1	**Downfolded Self-Energy of Many-Electron Systems and the Hubbard U** — •Ferdi Aryasetiawan
SYDF 1.2	Thu	15:15–15:45	H1	**LDA+Gutzwiller method for correlated electron systems** — •Zhong Fang
SYDF 1.3	Thu	15:45–16:15	H1	**Localized and itinerant states in *d*/*f*-electron systems unified by *GW*@LDA+*U*** — •Hong Jiang
SYDF 1.4	Thu	16:30–17:00	H1	**Giant polaronic effects in solids and nanstructures** — •Andrea Marini
SYDF 1.5	Thu	17:00–17:30	H1	**Excitation energies with time-dependent density *matrix* functional theory** — •Evert Jan Baerends, Klaas J. H. Giesbertz, Oleg Gritsenko, Katarzyna Pernal
SYDF 1.6	Thu	17:30–18:00	H1	**Calculations of multipoles in magnetic metals and insulators** — •Lars Nordström

Symposium Energy landscapes: Statistical physics of (spin-)glasses, biomolecules, clusters and optimization problems (SYEL)

See SYEL for the full program of the sympsium

SYEL 1.1	Mon	10:00–10:30	H1	**Energy Landscapes of clusters, glasses, and biomolecules** — •David Wales
SYEL 1.2	Mon	10:30–11:00	H1	**Order parameters and energy landscapes for protein folding and misfolding** — •Steven Plotkin
SYEL 1.3	Mon	11:00–11:30	H1	**Nuclear Spins Reveal the Microscopic Nature of Tunneling Systems in Glasses** — •Christian Enss
SYEL 1.4	Mon	11:30–12:00	H1	**Energy landscapes and phase transitions** — •Lapo Casetti
SYEL 1.5	Mon	12:00–12:30	H1	**Phase transitions in spin glasses** — •Peter Young
SYEL 1.6	Mon	12:30–13:00	H1	**Statistical physics of inverse problems** — •Riccardo Zecchina

Sessions

DF 1.1–1.3	Sun	16:00–18:15	H4	**Functional (oxide) single crystals and epitaxial films - from growth to function**
DF 2.1–2.6	Mon	11:00–13:00	H11	**Optical and nonlinear optical properties, photonic I**
DF 3.1–3.10	Mon	15:00–17:30	Poster D1	**Poster I: Nano- and microstructured dielectrics, surfaces and interfaces, dielectric composites**
DF 4.1–4.9	Mon	10:15–12:45	H3	**Multiferroics I (Joint Session of MA, DF, KR, DS)**
DF 5.1–5.14	Mon	14:00–17:45	H3	**Multiferroics II (Joint Session of MA, DF, KR, DS)**
DF 6.1–6.6	Tue	10:00–13:10	H11	**Focus Session: High-k and high mobility materials for CMOS**
DF 7.1–7.6	Tue	14:00–16:00	H11	**Dielectric and ferroelectric thin films**
DF 8.1–8.6	Tue	14:00–16:00	H9	**Electrical and mechanical properties**
DF 9.1–9.7	Wed	10:00–13:00	H11	**Focus Session: Structural dynamics in photoexcited molecules**
DF 10.1–10.9	Wed	14:00–17:30	H11	**Dielectric surfaces and interfaces**
DF 11.1–11.6	Wed	9:30–11:00	H8	**High-k and Low-k Dielectrics I (Joint Session DS/DF)**
DF 12.1–12.6	Wed	11:15–12:45	H8	**High-k and Low-k Dielectrics II (Joint Session DS/DF)**
DF 13.1–13.12	Wed	15:00–17:30	Poster A	**Poster II: Electrical, mechanical and optical properties, nonlinear dielectrics**
DF 14.1–14.11	Wed	14:00–17:30	H48	**Glasses I (Joint Session of DY, DF, CPP)**
DF 15.1–15.7	Thu	10:00–12:50	H11	**Optical and nonlinear optical properties, photonics II**
DF 16.1–16.3	Thu	14:00–15:25	H11	**Phase Transitions**
DF 17.1–17.6	Thu	15:30–17:30	H11	**Nano- and microstructured dielectrics**
DF 18.1–18.11	Thu	9:45–12:30	H38	**Glasses II (Joint Session of DY, DF, CPP)**

Annual General Meeting of the Dielectric Solids Division

Mittwoch 17:45–19:00 H11

- Bericht des Fachverbandleiters
- Tagungsnachlese
- Wahl des Fachverbandleiters
- Eingeladene Vorträge 2010
- Tutorial, Focus Sessions, Plenary Talks und Symposia 2011
- Verschiedenes

DF 1: Functional (oxide) single crystals and epitaxial films - from growth to function

Time: Sunday 16:00–18:15 Location: H4

Tutorial DF 1.1 Sun 16:00 H4

Influence of ferroelectric phase transitions on the melt growth of bulk oxide crystals — •Manfred Mühlberg and Manfred Burianek — Universität zu Köln, Institut für Kristallographie, Zülpicher Str. 49 b, 50674 Köln

Various applications in electronics, linear and nonlinear optics and other fields are connected with components taken from bulk single crystals. Also the determination of several fundamental physical properties like dielectric constants, piezo- or pyroelectric tensor components requires single crystalline samples. To meet these requirements one is primarily concerned with obtaining crystals of predetermined size with a high degree of structural perfection and a well-determined chemical composition.

In this introductory lecture, the most important growth methods from the melt and from high temperature solutions will be presented focusing on examples of selected ferroelectric perovskites and tetragonal tungsten bronzes. The chemical and thermophysical properties of the multi-component materials also represented by phase diagrams determine the synthesis steps and the details of the growth process.

A short overview of the defect types depending on the material properties and growth parameters will be given. Some options for reducing the defect content and improving the crystalline quality are reported for potassium lithium niobate and calcium barium niobate. Finally, a special attention is focused on the types and the influence of ferroelectric phase transitions being occuring between the growth temperature and the crystalline state at room temperature.

Tutorial DF 1.2 Sun 16:45 H4

Electromechanical properties of crystals — •Eiken Haussühl — Institut für Geowissenschaften / Abt. Kristallographie, Goethe Universität Frankfurt

The knowledge of physical properties of crystals as bulk materials is rather limited in comparison to the huge number of known crystal structures. In this introductory tutorial fundamental aspects of crystal physics will be presented. The lecture is intended to provide the basics for the understanding of the distinctiveness of crystalline compounds and to bring closer the phenomenological aspects under the influence of symmetry. It is also intended to highlight practical considerations for the measurement of selected tensorial properties. The main part will be focused on the mechanical properties of the bulk material like thermal expansion, elasticity and on electrical properties like piezoelectricity. Different effects arising from phase transition of selected organic and inorganic materials like oxides will be discussed.

Tutorial DF 1.3 Sun 17:30 H4

Epitaxial ferroelectric oxide thin films, nanostructures, and superlattices — •Dietrich Hesse, Ionela Vrejoiu, and Marin Alexe — Max Planck Institute of Microstructure Physics, Halle, Germany

Epitaxial ferroelectric thin films, nanostructures and superlattices represent a particularly interesting part of functional materials. In this tutorial, fundamental terms of epitaxial growth will be presented, along with a detailed characterization of growth-structure-property relations of a number of examples of perovskite-type ferroelectric structures. E.g., it will be shown how remanent polarization and switchability of pulsed-laser deposited Pb(Zr,Ti)O$_3$ (PZT) epitaxial thin films depend on the defect content (threading dislocations, stacking faults), and how the properties of antiferroelectric/ferroelectric PbZrO$_3$/PZT superlattices depend on the thickness of the individual layers via strain. The properties of epitaxial, ferroelectric (Bi,La)$_4$Ti$_3$O$_{12}$ nanostructures and Pt/PZT/Pt nanocapacitors of sub-100 nm size are shown to be determined by crystallographic orientation, crystal perfection, and size. The role of 2D defects will be highlighted, viz. ferroelectric 90 degree domain boundaries in epitaxial PZT films serving as nucleation centers for 180 degree switching, and the atomic structure of 180 degree boundaries influencing the switching process. Overall the interesting physical properties of epitaxial functional perovskite structures are discussed in terms of growth, crystal orientation, defect type, defect content, and strain.

DF 2: Optical and nonlinear optical properties, photonic I

Time: Monday 11:00–13:00 Location: H11

DF 2.1 Mon 11:00 H11

Relaxation dynamics of mixed phase and amplitude gratings attributed to optically excited small polarons in reduced LiNbO$_3$ — •Hauke Bruening, Raphael-Sung Hardt, Bettina Schoke, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The relaxation dynamics of elementary holographic gratings recorded with intense ns-laser pulses ($\lambda = 532\,\mathrm{nm}$, $\mathrm{I} = 350\,\mathrm{GW/m^2}$) is studied in thermally reduced, nominally undoped LiNbO$_3$ in the time regime of 10^{-8} s to 10^2 s at 785 nm. A stretched exponential decay of the diffraction efficiency is uncovered showing lifetimes in the ms-regime and a stretching coefficient $0{,}7 < \beta < 0{,}9$. By temperature dependent measurements, we can attribute the grating signal to probe light diffraction at a spatial density modulation of small bound $\mathrm{Nb}_{\mathrm{Li}}^{4+}$-polarons. Taking the presence of stable $\mathrm{Nb}_{\mathrm{Li}}^{4+}$:$\mathrm{Nb}_{\mathrm{Nb}}^{4+}$-bipolarons in the ground state into account, the density modulation is recorded via the optical gating mechanism. Remarkably, the initial value of the diffraction efficiency exceeds the expectation value for a pure c($\mathrm{Nb}_{\mathrm{Li}}^{4+/5+}$)-amplitude grating, i.e., the polaron density modulation is accompanied with a spatial modulation of the index of refraction. We discuss the origin of the phase grating in the frame of a microscopic model for polaron absorption and the presence of intrinsic photovoltaic currents.

*Financial support by the DFG (Projects IM37/5-1 and GRK 695) is gratefully acknowledged.

DF 2.2 Mon 11:20 H11

Numerical Investigations of Diffraction Efficiency of Two Center Holographic Recording in Photorefractive Crystals — •Mehmet Kiliç and Riza Demirbilek — Yildiz Technical University, Department of Physics, Davutpasa Campus, 34210 Esenler Istanbul Turkey

This contribution has been withdrawn.

DF 2.3 Mon 11:40 H11

Lasergepumpte Plasmaquelle für ultraschnelle zeitaufgelöste Röntgenbeugung — •Daniel Schick, Peter Gaal, Marc Herzog, Mareike Kiel, Steffen Mitzscherling, Wolfram Leitenberger und Matias Bargheer — Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam-Golm

Lasergepumpte Plasmaquellen eröffnen herausragende neue Möglichkeiten in der zeitaufgelösten Röntgenanalytik. Obwohl es sich bei der Plasmaquelle um ein kompaktes Table-Top System handelt, ist sie mit einer Pulsdauer von ca. 100 fs und einem Photonenfluss von 10^6 Photonen pro Sekunde am Probenort vergleichbar mit Femto-Slicing-Beamlines an Synchrotrons. Die neuartige Plasmaquelle an der Universität Potsdam verwendet ultrakurze, hochintensive Lichtpulse aus einem Titan-Saphir-Verstärker (30 fs, 7 μJ, 1 kHz), um harte Röntgenstrahlung zu erzeugen (Cu K_α). Dazu werden die Lichtpulse auf ein auf Spulen geführtes, 20 μm dünnes Kupferband fokussiert, so dass in einem Fokus von 2 μm Spitzenintensitäten von 10^{18} W/cm^2 erreicht werden. Für Pump-Probe-Experimente wird ein Teil der Ausgangsleistung des Lasers zum Anregen einer Dynamik in einer Probe verwendet. In einem Überblick zeigen wir erste Daten von zeitaufgelösten Röntgenbeugungsexperimenten an oxidischen Übergitterstrukturen.

DF 2.4 Mon 12:00 H11

Glass-ceramics as dielectrica for mobile applications in the GHz-range — •Stephan Knöner[1,2], Martin Letz[2], and Gerhard Jakob[1] — [1]Universität Mainz — [2]Schott AG , Mainz

There is an increasing number of mobile applications, which are working in the range of several GHz, for example GPS-handsets. Important elements of these applications are antennas, which have small dimensions and are working also in the direct vicinity of interfering dielectrica or lossy material, as for example a human body, which is called *body-loading*. Such a *body-loading* leads to detuning of resonances. One approach for solving this problem is to use a dielectric material to confine the electric-field component of the near-field of the antenna in a material so that the antenna characteristics show fewer changes under body-loading. The material, normally ceramics, for so called *Dielectric-Loaded Antennas* need to have several properties, as e.g. a large dielectric constant and a small dielectric loss. Besides having advantages in manufacturing, glass-ceramics obtained from a glassy phase are intrinsic pore free materials, which can be produced with high geometry accuracy. We present results of such glass-ceramics by leaning on known configurations of low loss GHz-ceramics, which were obtained.

DF 2.5 Mon 12:20 H11

Excitation Spectra of some AMX_3 Crystals and their Electronic Energy Levels — •Riza Demirbilek[1], Aysegül Çelik Bozdogan[1], Çigdem Elif Demirci[1], Gökhan Asan[1], Murat Çalişkan[1], and Gönül Özen[2] — [1]Yildiz Technical University, Department of Physics, Davutpasa Campus, 34210 Esenler Istanbul Turkey — [2]Istanbul Technical University, Department of Physics, Ayazaga Campus, 34469 Maslak Istanbul Turkey

This contribution has been withdrawn.

DF 2.6 Mon 12:40 H11

Excitation and Emission Spectra of $RbCdBr_3$-Crystal — •Aysegül Çelik Bozdogan[1], Murat Çaliskan[1], Gönül Özen[2], and Riza Demirbilek[1] — [1]Yildiz Technical University, Department of Physics, Davutpasa Campus, 34210 Esenler Istanbul Turkey — [2]Istanbul Technical University, Department of Physics, Ayazaga Campus, 34469 Maslak Istanbul Turkey

This contribution has been withdrawn.

DF 3: Poster I: Nano- and microstructured dielectrics, surfaces and interfaces, dielectric composites

Time: Monday 15:00–17:30 Location: Poster D1

DF 3.1 Mon 15:00 Poster D1

Lithium niobate nanoparticles: Orientation in externally applied electric fields* — •Bastian Knabe, Daniel Schütze, and Karsten Buse — Universität Bonn, Wegelerstr. 8, 53115 Bonn

The spontaneous polarization in lithium niobate leads to charged c-faces. It turns out that these surface charges of lithium niobate nanoparticles are not fully compensated. This leads to a remaining electrical dipole moment. We synthesize lithium niobate nanoparticles with a sol-gel method and measure their orientation in externally applied electric fields using this effect. By introducing dopants of different concentration and changing ambient conditions such as temperature, we investigate the various dependences of the dipole moment, which is generally about 10^{-3} of the dipole moment present for the uncompensated spontaneous polarization.

* Financial support by the Deutsche Forschungsgemeinschaft and the Deutsche Telekom AG is gratefully acknowledged.

DF 3.2 Mon 15:00 Poster D1

Formation and modification of Schottky barriers at the PZT/Pt interface — •Andreas Klein[1], Wenbin Wu[2], Feng Chen[1], and Robert Schafranek[1] — [1]Technische Universität Darmstadt, Institute of Material Science, Petersenstraße 32, D-64287 Darmstadt, Germany — [2]Hefei National Laboratory for Physical Science at the Microscale, University of Science and Technology of China, Hefei 230026, People's republic of China

A determination of the Schottky barrier height at the interface between ferroelectric Pb(Zr,Ti)O3 thin films and Pt using in-situ photoelectron spectroscopy is presented. The barrier height for holes, given by the energy difference of the valence band maximum and the Fermi energy, varies reversibly between 1.1 and 2.2 eV for oxidizing and reducing treatments. The changes in barrier are accompanied by a varying amount of metallic Pb at the interface. The most severe reduction is observed after storage in vacuum, which is attributed to the strongly reducing environment because of the presence of hydrogen and water in the residual gas of the vacuum system and the catalytically active Pt surface.

DF 3.3 Mon 15:00 Poster D1

DFT modelling of $SrO(SrTiO_3)_n$ Ruddlesden-Popper surfaces
— •Matthias Zschornak[1,2], Emanuel Gutmann[1], Torsten Weissbach[1,2], Tilmann Leisegang[1], Dirk C. Meyer[1,3], and Sibylle Gemming[2] — [1]Nachwuchsgruppe Nanostrukturphysik, Institute of Structural Physics, TU Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, Germany — [3]Institute of Experimental Physics, TU Bergakademie Freiberg, Germany

Strontium titanate ($SrTiO_3$) is an oxide crystallizing with cubic perovskite-type of structure that exhibits a high tunability of dielectric, electric, mechanical and optical properties by means of defects. Apart from dopants, also intrinsic oxygen vacancies or ordered stacking faults, e.g. Ruddlesden-Popper (RP) phases $SrO(SrTiO_3)_n$, may influence these properties.

We have investigated the surface energy, relaxation and electronic properties of such RP surfaces up to $n = 3$ in comparison to 'pure' $SrTiO_3$ by means of density-functional theory for $\langle 001\rangle$ and $\langle 100\rangle$ directions and with all possible perfect crystal terminations. We find a significant influence of the surface-near SrO-OSr stacking fault on surface energies and rumpling. Migrating surface states decrease the band gap of TiO_2 terminations but all terminations show insulating character. A detailed discussion of surface-near relaxations will be presented.

DF 3.4 Mon 15:00 Poster D1

Ferroelectric lithography: The promising route for assembling metallic and molecular nanostructures — •Alexander Haussmann, Mathias Schröder, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

The presence of different surface charges and thus different surface reactivities offers the possibility of exploiting domain-structured ferroelectrics as templates for assembling various functional nanostructures. This technique is claimed ferroelectric lithography [1], bearing the power for the controlled bottom-up assembly and integration of dissimilar species over large sample areas.

Here, we report on both the assembly and characterization of noble-metallic and molecular nanowires that were deposited photochemically at 180° domain walls on 5 mol% Mg-doped congruent $LiNbO_3$ single crystal templates [2]. By using different AFM techniques, the domain wall decoration was analyzed in detail with respect to the underlying domain structure (imaged by piezoresponse force microscopy, PFM). Furthermore, a promising explanation of this effect due to UV-induced domain wall conductivity will be discussed.

[1] S.V. Kalinin et al., *Nano Letters* **2**, 589 (2002).
[2] A. Haussmann et al., *Nano Letters* **9**, 763 (2009).

DF 3.5 Mon 15:00 Poster D1

Kohärente Phononen in oxidischen Materialien — •Peter Gaal, Daniel Schick und Matias Bargheer — Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam-Golm

Kohärente Phononen in Perovskit-Materialien lassen sich durch Impulsive Stimulierte Ramanstreuung (ISRS) erzeugen. In unserem Experiment werden zwei Replika eines ultrakurzen Lichtimpulses in verschiedene Kristalle (Strontium-Titanat, Barium-Titanat, etc.) und Multischichtstrukturen fokussiert. Durch Interferenz der beiden Lichtpulse wird ein transientes Gitter geschrieben, an dem ein dritter, zeitversetzter Lichtpuls gebeugt wird. Die beim Schreiben des transienten Gitters erzeugte kohärente Überlagerung unterschiedlicher Phonon-Polaritonen hängt in ihrer Energie und in ihrem Wellenvektor vom relativen Winkel sowie von der zeitlichen Dauer der interferierenden

Lichtimpulse ab. Damit lassen sich prinzipiell selektiv bestimmte Phononenbänder anregen. Mit dieser Methode können z.B. Phasenübergänge in oxidischen Materialien untersucht werden.

DF 3.6 Mon 15:00 Poster D1

Growth of TiO_x Thin Films by Liquid Delivery Atomic Layer Deposition for future RRAM Applications — •Marcel Reiners, Seong Keun Kim, Susanne Hoffmann-Eifert, Jiahua Zhang, Carsten Kuegeler, and Rainer Waser — Forschungszentrum Juelich, IFF-6 and JARA-FIT, 52425 Juelich, Germany

Titanium-dioxide ($TiO_{2-\delta}$) is widely studied as material for redox based resistive switching memories. The Atomic Layer Deposition (ALD) enables dense and 3D conformal films down to a thickness of a few nanometer. Here we report on liquid delivery ALD of TiOx from Titanium-tetramethylheptanedoinato-di-isopropoxide ($Ti(TMHD)_2(O\text{-}i\text{-}Pr)_2$) and Titanium-tetrapropoxide ($Ti(O\text{-}i\text{-}Pr)_4$) as precursors with water as oxygen source. The film growth was characterized by XRR and XRF and the morphology was analyzed by means of AFM and HRTEM. TiO_2 films prepared from $Ti(TMHD)_2(O\text{-}i\text{-}Pr)_2$ deposited on Pt|ZrO2|SiO2|Si in a temperature range from 340°C-390°C show a nanocrystalline anatase-type structure with a smooth morphology and a rms roughness about 0.1 nm. TiO_2 films deposited from $Ti(O\text{-}i\text{-}Pr)_4$ at a temperature of 250°C undergo a structural change from an amorphous to a polycrystalline phase above a critical film thickness of about 10 nm. Low current bipolar resistance switching was confirmed in 100x100 nm^2 small Pt|TiO_2|Ti|Pt structures with integrated 8 nm TiO_x films.

This work was supported by the Deutsche Forschungs Gemeinschaft (DFG, DE790/5-1 & HO2480/2-1).

DF 3.7 Mon 15:00 Poster D1

Investigation of the optical phonon modes of $BaTiO_3$ thin films using Raman scattering spectroscopy and IR spectroscopic ellipsometry — •Christian Kranert, Chris Sturm, Stefan Schöche, Rüdiger Schmidt-Grund, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The coupling of the switchable and non-switchable polarization of ferroelectric and pyroelectric materials in heterostructures results in new physical effects which can be used for modulators, sensors and, memories.[1] The properties of the ferroelectric polarization are strongly related to the phonon spectrum. In this work we present the investigation of the optical phonon modes of ZnO and $BaTiO_3$ and ZnO-$BaTiO_3$ heterostructures by Raman spectroscopy and infrared spectroscopic ellipsometry. A comparison of the phonon modes in heterostructures with those of single films provides access to the properties of the polarization interaction in these heterostructures.

The $BaTiO_3$ and ZnO thin films as well as the $BaTiO_3$-ZnO heterostructures were grown by pulsed laser deposition (PLD). The Raman measurements were carried out using two different lasers at a wavelength of 532 nm and 325 nm, respectively, in order to realize an excitation below as well as above the band gap of both the materials which allows to control the penetration depth of the probe-light in the films and heterostructures, respectively.

[1] O. Auciello and R. Ramesh, MRS Bull. Vol. **29**, No. 7 (1996)

DF 3.8 Mon 15:00 Poster D1

A theoretical description of constant phase element — •Mohammad Reza Shoar Abouzari[1], Frank Berkemeier[2], and Guido Schmitz[2] — [1]Department of Physics, Zabol University, Zabol, Iran — [2]Institut fuer Materialphysik, Wilhelm-Klemmstr. 10, 48149 Muenster

In most cases, the experimental results of impedance spectroscopy fit precisely to the parallel circuit of an Ohmic Resistance and a phenomenological Constant Phase Element (CPE) instead of a simple RC equivalent circuit. For this reason, this empirical model is widely used, but the physical meaning of the CPE is rarely discussed. We have introduced a physical interpretation of the CPE based on the Concept of Mismatch and Relaxation theory (CMR) of Funke et al. Complex impedance spectra of ion-conducting lithium borate network glasses are used to study the deformed shape of impedance semicircles which are usually described by a parallel circuit of R-CPE. Based on the CMR, we have introduced an equivalent circuit, named CMR-C model. It takes into account the contribution of the static glass network by introducing an additional capacitor. This model describes the experimental data accurately. Upon this model we found that the CPE can be considered to be equivalent to three basic elements, R(ω), C(ω), and C(inf) , which are defined by the parameters of the CMR.

DF 3.9 Mon 15:00 Poster D1

Fatigue in ferroelectric polymers: Polyvinylidene fluoride (PVDF) — •Jörg Schütrumpf, Sergej Zhukov, and Heinz von Seggern — Technische Universität Darmstadt, Darmstadt, Deutschland

A strong piezoelectricity, pyroelectricity and ferroelectricity in polyvinylidene fluoride (PVDF) made this polymer an object of detailed studies over the last 20 years. Ferroelectric polymers have an advantage over traditional ferroelectric materials due to their good mechanical properties. Although the stability of the ferroelectric polarization in PVDF is not satisfying for a wide range of applications, it still remains a model material for numerous studies on polarization and hysteresis phenomena in ferroelectric polymers. In order to gain a more systematic understanding of the polarization properties we performed fatigue experiments on 9 μm thin uniaxial stretched PVDF films. After bipolar stressing of the samples above the coercitive field strength E_c at frequencies from 50 Hz up to 10 kHz, switching curves and hysteresis loops were investigated. By comparing fatigued with unstressed samples the underlying effects of aging and fatigue are determined. We also report on the back-switched fraction of the polarization after an applied electric field is switched off with and without fatigue. Therefore the poling times are varied over nine decades for each electric field and the back-switched part during short-circuiting is measured at the end of each poling pulse.

DF 3.10 Mon 15:00 Poster D1

Experimental studies of dielectric constants in multi-layer systems — Axel Hommes[1], Christian Krebs[1], •Gört Luedtke[2], Dirk Nüssler[1], and Klaus Wandelt[2] — [1]Fraunhofer Institute for High Frequency Physics and Radar Techniques (FHR), Dep. mm-wave radar and high frequency sensors (MHS), Neuenahrer Straße 20, 53343 Wachtberg, Germany — [2]University of Bonn, Institute for Physical and Theoretical Chemistry, Dep. Surfaces and Interfaces, Wegeler Str. 12, 53115 Bonn, Germany

The results of experimental studies of the dielectric properties of multilayer systems and relevant absorption spectra will be presented. The measurements have been performed in the terahertz frequency range for different materials with varying layer thickness. Based on multi reflections in a multi layer structure, thickness measurement of single layers is a critical task for every measurement system. Reflections and interferences are unwanted influences during the measurement, but under well known conditions they can be utilized to characterize the layer thickness in multilayer structures. Based on the material parameters for the single layers like permittivity, attenuation etc. changes in the thickness of the different layers can be detected. An exact model of the multilayer structure is necessary including different attenuation coefficients, permittivities, etc. Based on this model changes in the layer thickness of the multilayer structure can be predicted. The estimation of layer thickness can be realized through continuous wave systems of the mmW or THz frequency range. The poster describes and compares modeling and first measurements with artificial structures.

DF 4: Multiferroics I (Joint Session of MA, DF, KR, DS)

Time: Monday 10:15–12:45 Location: H3

Invited Talk DF 4.1 Mon 10:15 H3

Antiferromagnetic interlayer coupling in $La_{0.7}Sr_{0.3}MnO_3$ / $SrRuO_3$ superlattices — •Ionela Vrejoiu — Max Planck Institute of Microstructure Physics, Halle, Germany

Perovskite oxides are versatile materials with a broad spectrum of physical properties, such as (anti)ferromagnetism, (anti)ferroelectricity, superconductivity, and multiferroicity. As illustrating examples, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and $SrRuO_3$ (SRO) are both ferromagnetic perovskites with bulk ferromagnetic Curie temperatures of 370 K and 160 K, respectively. LSMO is a 3d transition metal double exchange ferromagnet, whereas SRO is a rare case of a 4d itinerant metallic ferromagnet and, in contrast to LSMO, SRO shows exceptionally strong magneto-crystalline anisotropy. Such differences make the interlayer coupling between LSMO and SRO epitaxial thin films an intriguing case. We report on LSMO / SRO superlattices (SLs) grown by pulsed-laser deposition on vicinal TiO_2-terminated $SrTiO_3$ (100) (STO) substrates. These SLs exhibit strong antiferromagnetic (AF) interlayer coupling at temperatures below 140 K, where the SRO layers become ferromagnetic. SLs in which an ultrathin nonmagnetic perovskite spacer was grown in between all the LSMO and SRO layers (so that the LSMO and SRO have no mutual interfaces) exhibited ferromagnetic coupling below 140 K. This indicates that the AF coupling occurs only in SLs with direct interfaces between LSMO and SRO. A joint study of structural characterization, SQUID magnetometry as well as first principles calculations was performed, in order to unravel the origin of this strong AF coupling.

DF 4.2 Mon 10:45 H3

Magnetic phase transition at a biferroic interface predicted from first principles — •Michael Fechner[1], Igor Maznichenko[2], Sergey Ostanin[1], Arthur Ernst[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]MPI für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

The interface magnetoelectric effect mediates the change of the magnetization at a ferromagnetic/ferroelectric interface when the electric polarization is modified. Using first principle methods, we investigate different ultrathin ferromagnetic films (Co and Fe) on top of ferroelectric $ATiO_3$ (A=Pb,Ba) perovskites upon the occurrence of it. The calculations show that at the interface a moderately change of the size of the total magnetization takes place [1]. Further the magnetic ordering of the Fe film is sensitive to its thickness, so an unexpected antiferrimagnetic ordering appears for 2ML Fe whereas for all other thicknesses ferromagnetic ordering is preferred. Hybridization and strain effects at the interface can explain all observations. An interesting perspective for further studies will be the investigation of thin films of a CoFe alloy. This may allow gaining control of the magnetic ordering by the electric polarization.

[1] Fechner et al.. PRB 78, 212406(2008)

DF 4.3 Mon 11:00 H3

Magnetoelectric coupling at modified Fe/$BaTiO_3$ interfaces — •Martin Hölzer[1], Michael Fechner[2], Sergey Ostanin[2], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06900 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Two-component multiferroics are gaining attention within the last years. These compound materials, consisting of ferromagnetic and ferroelectric layers, combine the advantages (e. g. high curie temperatures) of their components in a tuneable magnetoelectric structure.

Ab initio DFT studies of ultrathin Fe films on ferroelectric $BaTiO_3$ show that their magnetoelectric coupling can be enhanced considerably by means of interface alloying.

In these systems, the magnetoelectric coupling is related to structural changes in the interface region under polarisation reversal of the $BaTiO_3$ substrate. In one of the considered cases, a magnetic phase transition with high change in the total magnetization is triggered under polarization reversal.

DF 4.4 Mon 11:15 H3

Towards ferroelectric tunneling barriers with magnetic electrodes — •Daniel Pantel, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The tunneling magnetoresistance (TMR) is a well-established quantum phenomenon in oxide electronics [1]. Recently, tunneling electroresistance was experimentally investigated in an oxide ferroelectric tunneling barrier [2, 3]. Combining both functionalities in one device, i.e. a ferroelectric barrier sandwiched in between two ferromagnetic electrodes, yields interesting properties, e.g. different effects of the ferroelectric polarization on the two spin channels [4]. However, experimental results are still lacking.

In this talk we report on the growth and the properties of perovskite oxide heterostructures consisting of a pulsed laser deposition-grown thin ferroelectric barrier layer sandwiched between two magnetic electrodes. First electrical measurements on capacitor-like tunneling junctions are presented.

[1] De Teresa, J.M., *et al.*, Science **286**, 507 (1999)
[2] Contreras, J.R., *et al.*, Appl. Phys. Lett. **83**, 4595 (2003)
[3] Garcia, V., *et al.*, Nature **460**, 81 (2009)
[4] Velev, J.P., *et al.*, J. Appl. Phys. **103**, 07A701 (2008)

DF 4.5 Mon 11:30 H3

Multiferroic materials with a non-collinear spin structure - A many-particle approach — •Thomas Michael[1], Julia M. Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Department of Physics, University of Sofia, Sofia, Bulgaria

Multiferroic bulk materials with a conical spin structure are investigated in the framework of a many-particle approach. The analysis of the ferroelectric subsystem is based on a two-state quantum model. Magnetic moments interact via the Heisenberg model. The canting of the spins is incorporated by the Dzyaloshinski-Moriya interaction. A representation of the spin operators with an arbitrary quantization axis is chosen. Minimizing the free energy yields the direction of the quantization axis. The multiferroic coupling term is discussed. A Green's function technique in reciprocal space provides the temperature dependence of the magnetization, polarization and the energy of the excitations.

DF 4.6 Mon 11:45 H3

Manipulating ferroelectric domains of multiferroic $DyMnO_3$ by soft X-rays — •Victor Soltwisch, Enrico Schierle, Detlef Schmitz, Dimitri Argyriou, Fabiano Yokaichiya, Ralf Feyerherm, and Eugen Weschke — Helmholtz Zentrum Berlin

In multiferroic $DyMnO_3$, ferroelectricity is induced by cycloidal magnetic structures of a chirality coupled to the direction of the electric polarization. XRMS at the Dy-M5 resonance allows to distinguish surface regions of different chirality of the Dy-4f magnetic cycloid and, hence, can be used to image ferroelectric domains. Furthermore, the x-ray beam itself can be utilized to manipulate the distribution of domains at the crystal surface.

DF 4.7 Mon 12:00 H3

Evidence of electro-active excitation of the spin cycloid in $TbMnO_3$ — •Alexey Shuvaev[1], Viktor Travkin[2], Vsevolod Ivanov[2], Alexander Mukhin[2], and Andrei Pimenov[1] — [1]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [2]General Physics Institute, Russian Academy of Science, 119991 Moscow, Russia

The coupling between the magnetic and ferroelectric orders in multiferroics is currently a topic of intense study. The materials of particular interest are those where the incommensurate cycloidal ordering of the spins drives the ferroelectricity. One of the consequences of multiferroicity is the existence of novel coupled magnon-phonon excitations called electromagnons. In addition to the electromagnon along the *a*-axis, the polarization analysis of the experimental spectra suggests the existence of an electro-active excitation for ac electric fields along the crystallographic *c*-axis. This excitation is possibly the electro-active eigenmode of the spin cycloid in $TbMnO_3$, which has been predicted within the inverse Dzyaloshinskii-Moriya mechanism of magnetoelectric coupling.

DF 4.8 Mon 12:15 H3

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations — •T. Finger[1], M. Baum[1], A. C. Komarek[1], D. Senff[1], P. Link[6], K. Hradil[5], K. Schmalzl[4], W. Schmidt[4], L.-P. Regnault[3], D. N. Argyriou[7], P. Becker-Bohaty[2], L. Bohaty[2], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln — [3]CNG-Grenoble / ILL, Grenoble — [4]FZ Jülich, JCNS at ILL, Grenoble — [5]Universität Göttingen / FRM2 München — [6]FRM2, TU München, München — [7]HMI, Berlin

We present neutron-scattering experiments on IN12 and on IN14 using spherical polarization analysis directly documenting the poling of the elastic magnetic chiral terms for the spiral magnets $MnWO_4$ and $TbMnO_3$ by cooling in an electric field. In addition, we were able to observe a multiferroic hysteresis curve as function of electric field in both compounds and succeeded to switch the spiral at constant temperature, which is the central issue in view of future applications. Additionally, measurements of the diffuse scattering slightly above the multiferroic transition show some small chiral terms remaining in the collinear phase. The close coupling of ferroelectricity and magnetism in the multiferroic materials also results in new collective excitations, predicted almost 20 years ago: hybridised spin-phonon excitations, referred to as "electromagnons". After the first observations of potential electromagnon modes in infra-red and in neutron studies a conclusive interpretation is still missing. Our most recent neutron scattering measurements will be discussed.

DF 4.9 Mon 12:30 H3

Topological magnetoelectric memory effect in the spin-spiral multiferroic MnWO$_4$ — •Dennis Meier[1], Naemi Leo[1], Thomas Lottermoser[1], Petra Becker[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Within the field of multiferroics, i.e. compounds with coexisting magnetic and electric order, so-called spin-spiral ferroelectrics attract tremendous attention. In these systems magnetic long-range order violates the inversion symmetry and induces a spontaneous electric polarization. Magnetic and electric domains are thus rigidly coupled so that "giant" magnetoelectric effects are obtained. However, up to now nearly nothing is know about the topology of the domain state in these systems. We report spatially-resolved measurements of the multiferroic domain topology in MnWO$_4$. For the first time, the full three-dimensional domain structure in a spin-spiral system is imaged. Our study reveals that the multiferroic domains in magnetically-induced ferroelectrics unify features that are associated to a magnetic domain state and others that point unambiguously to ferroelectric domains. Hence, a description in terms of ferroelectric or antiferromagnetic domains is incomplete and no longer appropriate. The novel concept of "multiferroic hybrid domains" is introduced. Annealing cycles reveal a topological memory effect: Due to phase coexistence at one phase boundary limiting the multiferroic state in MnWO$_4$, the entire multiferroic multidomain state can be reconstructed subsequent to quenching it. This work is supported by the DFG through SFB608.

DF 5: Multiferroics II (Joint Session of MA, DF, KR, DS)

Time: Monday 14:00–17:45 Location: H3

DF 5.1 Mon 14:00 H3

Switching of a spin-spiral-induced polarization in multiferroic MnWO$_4$ — •Tim Hoffmann[1], Dennis Meier[1], Petra Becker-Bohatý[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Coexisting ferroic orders become interesting when there is an interaction between them. Especially applying an electric field and thus changing the magnetic order is highly desirable for possible applications. In spite of the declared interest in multiferroics to switch a magnetization by an electric field nothing is known about the dynamics of the actual switching process.

The coupling of ferroelectric and magnetic order is intrinsically strong in spin-spiral multiferroics, where ferroelectricity emerges as a consequence of complex magnetic long-range order. Here we observe the manipulation of magnetically-induced ferroelectric domains in MnWO$_4$ by optical second harmonic generation (SHG). Application of an electric field allows to transform the sample to an electric as well as magnetic single-domain state. Moreover we obtained images of the domain structures during the transition revealing the growth of the domains. When cooled in zero-field, the domains have a bubble-like topology. Interestingly, after recovery from a single domain state the shape changes to a stripe structure and the domain size is significantly increased. Effects of the shape and duration of the electric-field poling pulses are investigated. Furthermore, in contrast to typical ionic ferroelectrics the spontaneous polarization can be switched without fatigue – no defects or pinning effects constrain the movement of domain walls.

DF 5.2 Mon 14:15 H3

Single Crystal X-ray diffraction studies on multiferroic YMn$_{2-x}$Fe$_x$O$_5$ — •Sven Partzsch[1], Jochen Geck[1], Norman Leps[1], Roberto Kraus[1], Dmitr Souptel[1], Bernd Büchner[1], and Enrico Schierle[2] — [1]IFW Dresden — [2]Helmholz-Zentrum Berlin

Temperature dependent single crystal X-ray diffraction studies of YMn$_{2-x}$Fe$_x$O$_5$ are presented. Upon cooling, the undoped material (x=0) orders antiferromagnetically below $T_\mathrm{N} \approx 45\,\mathrm{K}$ and becomes multiferroic below $T_{CE} \approx 39\,\mathrm{K}$. This multiferroic phase is destabilized rapidly with increasing Fe-content and we address here the reasons for this dramatic effect. The crystallographic study implies that the doped Fe mainly occupies the square pyramidal coordinated Mn position instead the octahedral one, which shows that these lattice sites are crucial for the MF properties.

In order to further characterize the electronic ordering in the ferroelectric phase of the undoped samples, we also applied soft resonant X-ray diffraction, which clearly shows that the oxygen states play an important role as well.

DF 5.3 Mon 14:30 H3

Electronic structure and magnetism in YFeMnO$_5$ — •Torsten Weissbach[1], Tilmann Leisegang[2], Axel Lubk[2], Dirk C. Meyer[3], and Sibylle Gemming[4] — [1]Inst. f. Theoretische Physik, TU Bergakademie Freiberg — [2]Inst. f. Strukturphysik, TU Dresden — [3]Inst. f. Experimentelle Physik, TU Bergakademie Freiberg — [4]Inst. f. Ionenstrahlphysik u. Materialforschung, Forschungszentrum Dresden

YFeMnO$_5$ crystallizes in the structure type of the orthorhombic RMn$_2$O$_5$ class of oxides. These show a series of antiferromagnetic phases with propagation vectors (1/2-δ, 0, 1/4+ϵ) below $T_N \approx 45$ K. For several of these phases, magnetism coexists with ferroelectricity. In YFeMnO$_5$, only one commensurable ferrimagnetic phase was found below $T_N = 165$ K, and ferroelectricity is absent. We apply crystallographic and quantum chemical methods to compare the Fe-substituted and the mangenese-only compounds. Diffraction experiments show slight displacements of the atom sites with increasing Fe content. The largest effects are related to crystal-field repulsion acting on the local metal 3d orbitals. The interaction between the magnetic metal ions is studied using DFT calculations starting with a bias magnetization of the atoms.

DF 5.4 Mon 14:45 H3

***Ab initio* calculations of the magnetic properties of perovskites under deformation** — •Igor Maznichenko[1], Corina Etz[2], Arthur Ernst[2], Martin Lüders[3], Ingrid Mertig[1,2], Zdzislawa Szotek[3], and Walter Temmerman[3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom

Materials with perovskite and perovskite-like structures demonstrate a broad spectrum of physical properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, metal-insulator transition, Jahn-Teller and other effects are observed in perovskites. These properties of the mentioned materials with the common formula ABO$_3$ are very sensitive to the type of the cations A and B. La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) is a strongly correlated 3d transition metal oxide with a Curie temperature (T$_C$) above RT (370 K). For other La/Sr ratios different types of antiferromagnetism are observed. Other perovskite, ruthenate SrRuO$_3$ (SRO) is a 4d ferromagnet with T$_C$ = 160 K.

Here we perform *ab initio* calculations for LSMO and SRO in ideal cubic, tetragonally distorted, and different orthorhombic structures. We focus on magnetic order and Curie temperature of the above mentioned structures in the different structural phases.

DF 5.5 Mon 15:00 H3

Electric field induced magnetization switching in strained EuO — •Marjana Ležaić, Konstantin Rushchanskii, Frank Freimuth, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

EuO is one of the rare materials combining a semiconducting gap and ferromagnetic ordering. Due to this property, EuO was suggested as a spin-filter in magnetic tunnel junctions [1]. It was shown that its ordering temperature T$_\mathrm{C}$ of 69 K can be increased further by doping with Gd [2], or by a reduction of the lattice parameter [3]. Recently, it has also been shown that a spin-polarized 2-dimensional electron gas can be formed at the EuO/LaAlO3 interface [4]. The list of properties that are not only interesting from the point of view of basic research, but also indicate possible applications, does not end here. A newly discovered property, ferroelectricity in strained EuO [5] puts this material into the class of multiferroics with relatively high T_C. Employing *ab-initio* calculations, we demonstrate how the ferroelectric property can be exploited in EuO films under tensile strain in order to achieve electric control of the magnetization direction.

[1] T. Santos and J. S. Moodera, Phys. Rev. B **69**, 241203 (2004).
[2] R. Sutarto, *et al*, Phys. Rev. B **80**, 085308 (2009).
[3] N. J. C. Ingle and I. S. Elfimov, Phys. Rev. B **77**, 121202(R) (2008).
[4] Y. Wang, *et al*, Phys. Rev. B **79**, 212408 (2009).
[5] E. Bousquet, N. A. Spaldin, Ph. Ghosez, arXiv:0906.4235v1.

DF 5.6 Mon 15:15 H3

Ferroelectric properties of $BiFeO_3$ thin films under mechanical stress — •Martin Hoffmann, Oliver Mieth, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Since ferroelectric properties (polarization, coercive field, etc.) of thin films can differ dramatically from the corresponding bulk values due to lattice-mismatch-induced strain, the systematic investigation of the impact of mechanical stress on the nm-length-scale is an indispensable step towards the general understanding of ferroic thin film physics.

In the present study, 150-nm-thick multiferroic $BiFeO_3$ films grown on (001)-oriented $SrTiO_3$ substrates were inspected with piezoresponse force microscopy (PFM) towards their ferroelectric domain distribution and their local ferroelectric hysteresis behavior under both tensile and compressive stress.

The systematic variation of the externally applied mechanical stress by substrate bending allowed us to compensate or to enhance the strain effect, which can be quantified by monitoring the coercive field as a function of the bending angle.

DF 5.7 Mon 15:30 H3

Strain effects in spinel ferrite thin films from first principles calculations — •Daniel Fritsch and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

We present density functional theory calculations of the structural and magnetic properties of the inverse spinel systems $CoFe_2O_4$ (CFO) and $NiFe_2O_4$ (NFO). Both are insulating magnets with high magnetic ordering temperatures and large saturation magnetization, which have been of particular interest over the past few years as building blocks of multiferroic heterostructures [1]. In order to effectively design the magneto-electric response of such multiferroic heterostructures, a clear picture of strain-induced changes in the magnetic properties of CFO and NFO is particularly important. Here we present results for the structural and magnetic properties of both CFO and NFO, with special emphasis on strain-induced changes in the magnetocrystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties.

[1] H. Zheng et al., Science 303, 661 (2004).

15 min. break

DF 5.8 Mon 16:00 H3

Mechanism of ferroelectric instabilities in non-d^0 perovskites: $LaCrO_3$ versus $CaMnO_3$ — Tim Harris, Roman Kovacik, and •Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The incompatibility of partial d occupation on the perovskite B-site with the standard charge transfer mechanism for ferroelectricity has been a central paradigm in multiferroics research [1]. Nevertheless, it was recently shown by density functional theory calculations that $CaMnO_3$ exhibits a polar instability that even dominates over the octahedral tilting for slightly enlarged unit cell volume [2]. Here, we present similar calculations for $LaCrO_3$, which has the same d^3 B-site electron configuration as $CaMnO_3$. We show that $LaCrO_3$ exhibits a similar, albeit somewhat weaker, volume-dependent polar instability as $CaMnO_3$, but while the Born effective charge (BEC) for the Mn^{4+} cation in $CaMnO_3$ is highly anomalous, the BEC for Cr^{3+} in $LaCrO_3$ is only slightly enhanced. We decompose the BECs for both systems in contributions of individual Wannier functions to elucidate the different driving force behind the polar instability in these systems.

[1] N. A. Hill, J. Phys. Chem. B 104, 6694 (2000). [2] S. Bhattacharjee et al., Phys. Rev. Lett. 102, 117602 (2009).

DF 5.9 Mon 16:15 H3

Multiferroicity in $EuTiO_3$ and $Eu_{1-x}Ba_xTiO_3$: *ab initio* characterization of crystalline, magnetic and electronic structure — •Konstantin Z. Rushchanskii[1], Marjana Ležaić[1], and Nicola A. Spaldin[2] — [1]Institut für Festkörperforschung, Quanten-Theorie der Materialien, Forschungszentrum Jülich GmbH, 52425 Jülich, and JARA-FIT, Germany — [2]Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

We report a systematic study of possible structural transitions in $EuTiO_3$ and ordered $Eu_{1-x}Ba_xTiO_3$ mixed compounds. We investigated phonon spectra of $EuTiO_3$ and found strong M- and R-point instabilities, indicating antiferrodistortive structural deformations. In the ordered $Eu_{0.5}Ba_{0.5}TiO_3$ compounds, the antiferrodistortive deformation is replaced by significant ferroelectric distortions, involving not only Ti, but also the magnetic Eu cation. We will discuss several scenarios of ferroelectric and antiferrodistortive transitions and their coupling with the magnetic structure. Corresponding changes in the phonon structure will be compared with available experimental data.

DF 5.10 Mon 16:30 H3

Electronic and magnetic properties of $LuFe_2O_4$ — •Karsten Kuepper[1], Michael Raekers[2], Christian Taubitz[2], Manuel Prinz[2], Christine Derks[2], Manfred Neumann[2], Andrei V. Postnikov[3], Frank M. F. de Groot[4], Cinthia Piamonteze[5], Dharmalingam Prabhakaran[6], and Stephen J. Blundell[6] — [1]Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [3]LPMD, Paul Verlaine University and Institute Jean Barriol, Metz, France — [4]Department of Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, 3584 CA Utrecht, Netherlands — [5]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [6]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

$LuFe_2O_4$ is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of $LuFe_2O_4$ are investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. We identified the electronic states of the valence band by means of valence band XPS-, and XES-spectroscopies, and GGA+U first principles calculations. Moreover, by applying XMCD, we are able to identify the spin ground state of $LuFe_2O_4$ in the charge ordered phase to be a 2:1 ferrimagnetic configuration, ruling out a frustrated magnetic state.

[1] K. Kuepper et al., Phys. Rev. B, Rapid Commun., in press.

DF 5.11 Mon 16:45 H3

Influence of Fe-substitution in $LiNi_{(1-x)}Fe_xPO_4$ on the antiferromagnetic structure — •Elke Künzel[1], Anne Zimmermann[1], Jiying Li[2], David Vaknin[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Ames Labatory and Department of Physics, Iowa States Univerity, Ames, USA

The $LiMPO_4$ system (M=Fe, Ni, Co, Mn) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds. In spite of their structural similarity, drastic differences in the domain topology are observed by optical SHG. Domains in $LiNiPO_4$ form anisotropic platelets whereas in $LiFePO_4$ they are isotropic and amoeba-like. It is yet unclear whether this surprising behaviour is due to the properties of the nickel ion or to the spin direction which points along z in $LiNiPO_4$ and along y in $LiFePO_4$.

In order to clarify this, samples with different mixing ratios of nickel and iron were studied. The domain structure of $LiNiPO_4$ was found to become aboeba-like for an iron substitution of «50%. An anomalous temperature dependence of the AFM order parameter and indications for a spin structure different from that of the end compounds was observed.

DF 5.12 Mon 17:00 H3

Non-Resonant Magnetic X-ray Scattering on Rare-Earth Iron Borates $RFe_3(BO_3)_4$ — •Jorge E. Hamann-Borrero[1], Martin Philipp[1], Olga Kataeva[2], Martin von Zimmermann[3], Christian Hess[1], Ruediger Klingeler[1], Alexander Vasiliev[4], Leonard Bezmaternykh[5], and Bernd Buechner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]A.E.Arbuzov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences, Kazan, Russia — [3]HASYLAB at DESY, Hamburg, Germany. — [4]Low Temperature Physics department, Faculty of Physics, Moscow State University, Moscow, Russia. — [5]L.V Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia.

Non-resonant magnetic XRD (NRMXRD) experiments with photon energy of 100keV where performed on selected compounds of the $RFe_3(BO_3)_4$ family as a function of temperature and applied magnetic field. The results show the existence of several unexpected diffraction features, in particular the presence of a magnetic super-lattice peak, and the appearance of two reflections that violate the diffraction conditions for the low temperature phase $P3_121$ of the iron borates. The magnetic nature of the former is concluded from analysing the scattering cross section at high energies and the magnetic structure of the different compounds. It is shown that the magnetic reflection reveals the magnetic properties of the material. For $GdFe_3(BO_3)_4$, values for the component of the spin moment perpendicular to the scattering plane ($S_\perp$) have been determined as well as the angle between the spin moment and the hexagonal basal plane.

DF 5.13 Mon 17:15 H3

Electronic structure, magnetic and dielectric properties of the edge-sharing copper-oxide chain compound NaCu2O2 — •Philippe Leininger[1], Martin Rahlenbeck[1], Markus Raichle[1], Britta Bohnenbuck[1], Andrey Malyuk[2], Chengtian Lin[1], Bernhard Keimer[1], Eugen Weschke[2], Enrico Schierle[2], Shinichiro Seki[3], Yoshi Tokura[3], and John Freeland[4] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin, Germany — [3]University of Tokyo, Dept. of Applied Physics, Bunkyo-ku, Tokyo 113-8656, Japan — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

We report an experimental study of NaCu2O2, a Mott insulator containing chains of edge-sharing CuO4 plaquettes, by polarized x-ray absorption spectroscopy (XAS), resonant magnetic x-ray scattering (RMXS), magnetic susceptibility, and pyroelectric current measurements. The XAS data show that the valence holes reside exclusively on the Cu2+ sites within the copper-oxide spin chains and populate a d-orbital polarized within the CuO4 plaquettes. Our results also demonstrate a new orbital selection rule for RMXS that is of general relevance for magnetic structure determinations by this technique. Dielectric property measurements reveal the absence of significant ferroelectric polarization below TN, which is in striking contrast to corresponding observations on the isostructural compound LiCu2O2. The results are discussed in the context of current theories of multiferroicity.

DF 5.14 Mon 17:30 H3

Magnetoelectric effect in diluted antiferromagnet $PbFe_{0.5}Nb_{0.5}O_3$ — •Vladimir Shvartsman[1], Pavel Borisov[2], Wolfgang Kleemann[2], and Antoni Kania[3] — [1]Institut für Materialwissenschaft, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Essen, Germany — [2]Angewandte Physik, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [3]Institute of Physics, University of Silesia, Katowice, Poland

Multiferroics, i. e. materials where two primary ferroic order parameters of magnetic and electric nature coexist, are of significant scientific and practical interest nowadays. Especially attractive are the multiferroics with enhanced magnetoelectric (ME) properties, which relate changes of polarization/magnetization to external magnetic/electric fields, respectively. While the linear ME effect has strong symmetry requirements and is rare, higher order ME couplings are allowed in all multiferroics. We report on investigations of magnetic and ME properties of (001)-oriented $PbFe_{0.5}Nb_{0.5}O_3$ (PFN) single crystals in the temperature range 5-300 K. PFN is ferroelectric below 385 K and antiferromagnetic below the Néel temperature, T_N=154 K. Temperature dependences of the magnetization exhibit a step like anomaly at T_N and a maximum on zero-field cooled curves at 8 K. Below T_N, the system manifests a spontaneous second order ME effect (electrobimagnetic effect), which reaches a peak value around 20 K. Moreover, after field cooling the linear ME effect has been observed, which disappears above 8 K. The nature of the low-temperature magnetic anomaly and the temperature dependences of the ME effects are discussed.

DF 6: Focus Session: High-k and high mobility materials for CMOS

Time: Tuesday 10:00–13:10 Location: H11

Invited Talk DF 6.1 Tue 10:00 H11

Gate Oxides beyond SiO_2 and the High K Materials Revolution — •Darrell Schlom — Department of Materials Science and Engineering, Cornell University, USA

A major materials milestone has been achieved that transforms the materials makeup of silicon-based field-effect transistors: the SiO_2 gate dielectric has been replaced by a hafnium-based dielectric in microprocessors produced by leading manufacturers. The incredible electronic properties of the SiO_2/silicon interface are the reason that silicon has dominated the semiconductor industry and helped it grow to over 250 billion US dollars in annual sales. The shrinkage of transistor dimensions has led to tremendous improvements in circuit speed and computer performance. At the same time, however, it has also led to exponential growth in the static power consumption of transistors due to quantum mechanical tunneling through an ever-thinner SiO_2 gate dielectric. This spurred an intensive effort to find an alternative to SiO_2 with a higher dielectric constant (K) to temper this exploding power consumption and enable Moore's law to continue. In this talk the comprehensive materials analysis to identify silicon-compatible materials that go beyond SiO_2 (i.e., with higher K and sufficient bandgap) will be described, together with how these materials have enabled improvements in MOSFETs, DRAM, and emerging semiconductor devices.

5 min. break

Topical Talk DF 6.2 Tue 10:45 H11

Advanced CMOS transistor technologies using HKMG and strained Silicon for high performance applications — •Manfred Horstmann — Globalfoundries Dresden

In this paper we present an overview about CMOS transistor technologies for advanced circuit applications. To achieve a *high performance per watt* figure of merit, transistor technology elements like strained Si, aggressive junction scaling and high K metal gate technology need hand-in-hand development with multiple core- and power efficient designs. These techniques have been developed, applied and optimized for 45nm volume manufacturing and are currently in ramp for the 28 & 32nm "Foundry" technology nodes at GLOBALFOUNDRIES in Dresden. Different High K metal gate integration schemes and their advantages for different circuit applications will be discussed. An outlook on 22nm technology will be given.

Topical Talk DF 6.3 Tue 11:10 H11

Amorphous ternary high-k oxides on Si and higher mobility substrates — •Marcelo Lopes[1,2], Eylem Durgun-Ozben[1,2], Alexander Nichau[1,2], Roman Luptak[1,2], Martin Roeckerath[1,2], Juergen Schubert[1,2], and Siegfried Mantl[1,2] — [1]Institute for Bio- and Nanosystems (IBN1), Research Center Juelich, Juelich, Germany — [2]JARA-Fundamentals of Future Information Technologies, Juelich, Germany

The miniaturization of metal-oxide-semiconductor field effect transistors (MOSFETs) is approaching fundamental limits. Novel materials are needed in order to continue the CMOS scaling. High-k dielectrics combined with semiconductors with better transport properties than Si is an attractive alternative. Strained Si (sSi), Ge, and SiGe are candidates with intrinsic higher carrier mobilities than Si. However, one of the issues that still remains is the challenge to achieve a high quality interface between the high-k film and these semiconductor substrates. The search for alternative high-k oxides that could offer stable interfaces offering a low density of electrically active defects has become a topic of major interest. Ternary rare earth oxides such as the scandates ($LaScO_3$, $GdScO_3$ or $DyScO_3$) and $LaLuO_3$ have been identified as promising high-k candidates for Si-based CMOS applications. In this contribution, we will review our results on the structural and electrical properties of $REScO_3$ (RE = La, Gd, Tb, Sm) and $LaLuO_3$ amorphous thin films deposited on Si. In addition, the integration of these oxides with high mobility substrates such as sSi, Ge, and SiGe will be presented.

Invited Talk DF 6.4 Tue 11:35 H11

Aspect Ratio Trapping: A Heterointegration Solution for Ge and III-V CMOS — •James Fiorenza — AmberWave Systems, Salem, NH, USA

Enhanced MOSFETs using high mobility non-silicon channel materials are being intensively investigated for future CMOS nodes. This research path is extremely promising, but significant challenges remain. Perhaps the largest challenge is the heterointegration of the high mobility materials with silicon. A heterointegration technique called Aspect Ratio Trapping (ART) is well suited to the unique integration requirements of mobility-enhanced CMOS. This technique involves epitaxial growth in narrow (< 500 nm), high aspect ratio silicon dioxide trenches. Threading dislocations generated by the lattice mismatch between the epitaxial material and silicon are trapped by the sidewalls of the trenches, greatly reducing the surface dislocation density. This technique been shown to be effective with a variety of relevant cubic semiconductors including Ge, InP and GaAs. The resulting buffer layers can be thinner than 500 nm, more than an order of magnitude thinner than traditional graded buffer heterointegration approaches, a critical advantage for CMOS applications.

5 min. break

Topical Talk DF 6.5 Tue 12:20 H11

Wafer Bonding Techniques for Advanced CMOS — •Manfred Reiche — Max-Planck-Institut für Mikrostrukturphysik, Halle

There are numerous discussions on future strategies of complementary metal-oxide-semiconductor (CMOS) device scaling. According to simulations, the gate length of an ultimately scaled MOSFET is well below 10 nm. Devices with gate lengths as small as 10 nm were already demonstrated using existing technologies. Apart from scaling new materials are employed to boost the transistor performance. Besides new materials for gate stacks (high-k materials, metal gates), interconnects, etc., new substrates are strongly required. For instance, silicon-on-insulator (SOI) is one of the most important substrates for high performance applications. The combination of the advantages of SOI with high-mobility channel materials (strained silicon, germanium) offers additional possibilities to improve the device performance. All these substrates are realized by wafer bonding techniques. The different wafer bonding techniques and their fundamental physical and chemical principles as well as the application to advanced CMOS substrates are reviewed.

Topical Talk DF 6.6 Tue 12:45 H11

Si wafer engineering: single crystalline oxides as buffers for the integration of alternative semiconductors — •Alessandro Giussani[1], Peter Zaumseil[1], Olaf Seifarth[1], Markus Andreas Schubert[1], Peter Storck[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]SILTRONIC AG, Hanns-Seidel-Platz 4, 81737 Muenchen, Germany

Single crystalline oxides are the object of intensive research as buffers for the integration of functional semiconductors on the mature Si platform. The interest is motivated on the one hand by the demand for cheap semiconductor substrates (i.e. Ge & GaN) on Si, and on the other hand by CMOS semiconductor (i.e Si & Ge)-on-insulator technologies. The main advantage of the oxide templates is the high flexibility to tune important epitaxy parameters of the overgrowing semiconductor. Bixbyite-based heterostructures are used by our group for Si, Ge and GaN integration. In the talk, special attention will be dedicated to solid solutions of (Pr2O3)1-x(Y2O3)x (x = 0-1) heterostructures which can be used for the growth of lattice-matched and -mismatched SiGe systems. As an example, pure Ge thin film heterostructures on cubic Pr2O3 are demonstrated. The grown Ge epilayers are single crystalline, atomically smooth and free of impurities from the buffer and Si. Moreover, a complex characterization of the Ge epilayer defect structure is presented by a combination of XRD and TEM.

DF 7: Dielectric and ferroelectric thin films

Time: Tuesday 14:00–16:00 Location: H11

DF 7.1 Tue 14:00 H11

Electrode polarization from a different point of view — •Björn Martin and Herbert Kliem — Saarland University, Germany

To investigate electrode and space charge effects thin film capacitance structures using ion-conducting polyethylene oxide contacted with metal electrodes are prepared.

In contrast to continuum models a discrete three-dimensional model is developed to describe the ionic motion. Single charges are regarded. Negative ions can fluctuate thermally activated over energy barriers in a multiwell potential. Positive immobile ions provide charge neutrality. Interactions of the ions with the electrodes using the method of images and all other electrostatic interactions are considered.

In simulations a coulombic attraction between the mobile ions and their image charges in the electrodes is found even in short circuit condition. The accumulated ions trapped at the electrodes together with their image charges yield dipole like fields repelling further ions towards the volume of the samples leaving behind a positive depletion zone. Thus, a maximum of the internal potential results in the middle of the sample which is verified experimentally.

With applied voltage the ions are partly detrapped. The mobile ions are shifted to the positive electrode and a broad depletion zone with positive immobile charges arises at the negative electrode. Therefore, a high potential drop is found here. In the bulk the potential increases only slightly indicating no space charges in this region.

DF 7.2 Tue 14:20 H11

Non-Kolmogorov-Avrami-Ishibashi switching dynamics in nanoscale ferroelectric capacitors — •Yunseok Kim[1], Hee Han[2], Woo Lee[3], Sunggi Baik[2], Dietrich Hesse[1], and Marin Alexe[1] — [1]Max Planck Institute of Microstructure Physics, D-06120 Halle (Saale), Germany — [2]Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang 790-784, Republic of Korea — [3]Korea Research Institute of Standards and Science (KRISS), Daejeon 305-340, Republic of Korea

The electrical polarization in ferroelectrics has two stable states which can be switched by applying an external electric field. The polarization switching mechanisms in macroscopic systems are usually treated within the framework of nucleation and growth theory, i.e. the Kolmogorov-Avrami-Ishibashi (KAI) model. Although there have been many efforts to understand switching dynamics, there is still lack of information on the switching dynamics mostly on nanoscale systems. The switching dynamics of nanoscale capacitors different from their macroscopic counterparts.Moreover, direct studies on nanoscale capacitors remain a challenge. Here we present switching dynamics of nanoscale capacitors with a radius of 35 nm using piezoresponse force microscopy. Polarization switching starts with only one nucleation event occurring only at a pre-determined place. The switching dynamics of nanoscale capacitors do not follow the classical KAI model. Based on the consideration of two separate (nucleation and growth) steps within a non-statistic finite system, we propose a new non-KAI model which is in good agreement with the experimental results.

DF 7.3 Tue 14:40 H11

Nonlinear Frequency Response of Ferroelectric Thin Films — •Kay Barz, Martin Diestelhorst, and Horst Beige — Martin Luther-Universität Halle-Wittenberg

The dielectric properties of ferroelectric thin films are commonly studied by means of low-frequency or quasi-static methods (capacitance-voltage, current-voltage, hysteresis). We pursue a different approach by investigating the frequency response of a LCR series-resonant circuit containing a ferroelectric thin film as capacitance. The talk presents amplitude-frequency responses observed at different types of thin film samples (Metal/Oxid,Semiconductor (MOS), Metal/Ferroelectric/Metal (MFM), Metal/Ferroelectric/Semiconductor (MFS)).

The results on MFM structures show, how hysteresis and its transient alterations due to fatigue manifest in a shift of resonance frequency under increasing or decreasing driving amplitude. In the circuit configuration used to obtain the time series data, the MOS and MFS structures become electrostatically charged by the ac amplitude. In case of the MFS capacitor, in this charged state, a strange nonchaotic attractor can be observed. Thus, ferroelectric thin films and ferroelectric/semiconductor heterostructures provide experimental access to some interesting phenomena known from theory of nonlinear dynamics.

DF 7.4 Tue 15:00 H11

Study of P3HT/PCBM based films by NEXAFS — •Matthias Richter, Daniel Friedrich, Shine Philip, Ioanna Paloumpa, Klaus Mueller, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

In this contribution we report on investigations of the electronic structure and composition of regioregular poly(3-hexylthiophene) (P3HT) and phenyl-C_{61}-butyric acid methyl ester (PCBM) based films by using Near Edge X-Ray Absorption Fine Structure (NEXAFS). The measurements were done at the U49/2-PGM2 beam line of BESSY II, Berlin using TEY (total electron yield) and TFY (total fluorescence yield) detection. The samples were produced by spin casting a mixture of P3HT (dissolved in chloroform) and PCBM (dissolved in chlorobenzene) on ITO (indium tin oxide) coated glass slides. Measurements of pure P3HT and PCBM show all typical excitations, whereas the blended system is a weighted superposition of the related peaks. Analyzing these weighted superposition, we observe in the surface sensitive TEY data an accumulation of P3HT, whereas in the bulk sensitive TFY signal an as expected mixture is found. We also show angular dependent NEXAFS measurements of the P3HT/PCBM blend in order to measure the orientation and distribution of the P3HT polymer. Additionally, we will show a new approach for organic solar cell application by introducing ferroelectric nanoparticles into the mixture.

DF 7.5 Tue 15:20 H11

Untersuchungen zum elektrischen Durchschlag in weichen Elastomermaterialien — •Matthias Kollosche, Hristiyan Stoyanov und Guggi Kofod — Universität Potsdam, Potsdam, Deutschland

Der Einfluss von Materialeigenschaften auf das elektrische Durchschlagsverhalten in weichen Materialien ist von vielfältigen Interesse bei der Verwendung von Smart Materials. Durch die Verwendung von Mischungen aus zwei chemisch identischen thermoplastischen Elastomeren gelingt eine Variation der Materialeigenschaften bei konstanter Temperatur, ohne zusätzliche Wechselwirkungen. Kraft-Dehnungs Versuche belegen die Möglichkeit einer kontinuierlichen Variation des Youngs Moduls durch die gezielte Wahl des Massenverhältnisses der Elastomermaterialien. Für die Ausführung der elektrischen Durchschlagsversuche wurden die Elastomermaterialien in Lösung und anschließend auf einem Glasträger mit Elektrode gebracht und getrocknet. Die Untersuchungen an den präparierten Polymerfilmen zeigen die Abhängigkeit der Durchbruchsfeldstärke von den mechanischen Eigenschaften des verwendeten Polymerfilms. Diese Ergebnisse werden mit dem ursprünglichen Modell zur elektromechanischen Instabilität von Garton-Stark und dem Modell von X. Zhao und Z. Suo (Appl. Phys. Lett. 95, 031904 (2009)) verglichen und ein verbesserter Ansatz zur Materialbeschreibung präsentiert. Das vorgeschlagene Modell ermöglicht, durch die Verwendung des hyperelastischen Materialansatzes und angepasster Randbedingungen, eine Beschreibungsmöglichkeit für den elektrischen Durchschlag in weichen Materialien

DF 7.6 Tue 15:40 H11

$CaTiO_3$ as a high-k dielectric in thin MIM Capacitor stacks — •Andreas Krause[1], Walter M. Weber[1], Andreas Jahn[2], Ulrich Merkel[2], Matthias Albert[2], Uwe Schroeder[1], Johann W. Bartha[2], and Thomas Mikolajick[1] — [1]namlab gGmbh, D-01187 Dresden — [2]Institut fuer Halbleiter- und Mikroelektronik IHM, TU Dresden

With the further increase in integration density of microelectronics, ordinary SiO_2-based dielectrics reach their limits as leakage currents increase significantly. Therefore, dielectric materials are required that combine a high dielectric constant (k) and low leakage currents. Metal Insulator Metal (MIM) stacks with the perovskite calcium titantate ($CaTiO_3$) as a high-k oxide were sputter deposited with variing thicknesses and deposition temperatures. As electrodes, different work function materials were used: Pt, Ru, TaSiN, TiN. Optimizing the roughness and deposition parameters of the electrodes, a k-value of 51 is reached with a capacitance equivalent thickness targeting 1nm. The leakage currents for 15 nm thick $CaTiO_3$ films are about $1 \cdot 10^{-7} A/cm^2$ at 1 V, which is in agreement with the ITRS roadmap of 2013. The morphology was studied with atomic force microscopy and scanning electron microscopy. Capacitor-voltage measurements were performed to extract the k-value. In addition, the crystallinity of the oxide and metal electrode was investigated with variable temperature x-ray defraction measurements, showing clearly the transition from the amorphous to the crystal state in dependence of the temperature.

DF 8: Electrical and mechanical properties

Time: Tuesday 14:00–16:00 Location: H9

DF 8.1 Tue 14:00 H9

High-pressure single-crystal structure investigations of sillenites — •Leonore Wiehl, Alexandra Friedrich, Eiken Haussühl, Wolfgang Morgenroth, and Björn Winkler — Institut für Geowissenschaften, Goethe-Universität, Frankfurt/Main, Germany

Sillenites, $Bi_{12}MO_{20}$ (M = Si, Ge, Ti), crystallize in the cubic noncentrosymmetric space group $I23$. They are piezoelectric and optical active, show an electro-optic effect and a high photoconductivity, leading to applications using the photorefractive effect. It is assumed, that some characteristics of these properties are correlated with the stereochemical activity of the $6s^2$ lone electron pair of Bi^{3+}.

At ambient conditions the Bi^{3+} lone pairs are oriented towards large cavities in the crystal structure of sillenites. Thus the stereochemical activity is expected to decrease, or even vanish, if the cavities are compressed under high external pressure. The crystal structures of $Bi_{12}SiO_{20}$, $Bi_{12}GeO_{20}$ and $Bi_{12}TiO_{20}$ were investigated at high pressure in diamond anvil cells. Single crystal X-ray intensity data were collected at ambient conditions in house and at pressures up to 16.8(3) GPa with synchrotron radiation at HASYLAB (D3).

We found the largest compression of interatomic distances along the lone pair directions. A complete collapse of the cavities, however, seems to be prevented by the high symmetry of the crystals. Changes of the $Bi^{[5+2]}O_7$ polyhedra will be discussed.

Financial support from the DFG (HA 5137/3-1) and from HASYLAB is gratefully acknowledged. We thank HASYLAB for synchrotron beamtime and Martin Tolkiehn for assistance at D3.

DF 8.2 Tue 14:20 H9

Space-charge wave excitation by static and moving interference patterns in $Bi_{12}GeO_{20}$ — •Burkhard Hilling, Thomas Schemme, Kay-Michael Voit, Heinz-Jürgen Schmidt, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

We report on space-charge wave (SCW) excitation in semi-insulating materials by simultaneous exposure with a static and a moving interference pattern and the application of a static electric field [1]. The two patterns with equal spatial frequency are generated independently from each other using a four-beam interferometer with only one light source. A single crystal of BGO ($Bi_{12}GeO_{20}$) was applied as an example; the investigations were performed at a wavelength of 514 nm using a total light intensity of 30 mW/cm^2, spatial frequencies of $(0.5 - 12) \cdot 10^3$ cm^{-1}, and electric fields ≤ 10 kV/cm. This method enables us to determine the sign of the charge carriers participating in SCW formation. Compared to the classical method using an oscillating interference pattern, this method increases the quality factor of the excited SCW [1]. The latter enabled studies with samples of thicknesses $d = 0.12 - 2.0$ mm cut from the same boule. Also the dependence of the SCW-signal on the direction of the electric field with respect to the crystallographic axes is studied. Remarkably, SCW excitation is independent from the sample's thickness and the orientation of the crystallographic axes. Hence, we can suggest, that it can be applied also to very thin samples ($d \ll 1$ μm), e.g., to semiconductor films. Financial support from the DFG (GRK 695) is gratefully acknowledged.

[1] B. Hilling *et al.*, PRB **80**, 205118 (2009)

DF 8.3 Tue 14:40 H9

Ab initio simulation of copper dopants and vacancies in the lead-free ferroelectric potassium sodium niobate — •Sabine Körbel and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg

Lead-free ferroelectric ceramics, for instance the perovskite potassium sodium niobate (KNN), are regarded as potential future alternatives to the widely used lead zirconate titanate (PZT) for piezoelectric applications. These materials can be doped with various elements in order to optimize their ferroelectric properties for the respective application. In the case of KNN, copper oxide can be added during processing as a sintering aid.

In this work, the influence of metal impurities on the ferroelectric properties of KNN is investigated for the example of Cu. By means of ab initio density functional theory, we determined the prevailing point defect types and the preferred lattice sites of Cu dopants for different processing conditions, and the stability of dopant-vacancy complexes.

In order to study the influence of point defects on switching the ferroelectric polarization of KNN, we investigated the effect of Cu on the energy needed for switching between different polarization directions.

DF 8.4 Tue 15:00 H9

Planar defects and dislocations in perovskite materials — •Pierre Hirel[1], Matous Mrovec[1,2], and Christian Elsaesser[1,2] — [1]Institut für Zuverlässigkeit von Bauteilen und Systemen (IZBS), Universität Karlsruhe (Germany) — [2]Fraunhofer Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg im Breisgau (Germany)

Plastic deformation, which depend on extended defects properties, can have dramatic influence on the electronic, optical and mechanical behavior of materials. In perovskite-type ceramics, which are functional components of electroactive devices, lattice dislocations are known to have an important influence on the devices' performance and lifetime. In the case of confined systems (e.g. epitaxial thin films, superlattices, nanoparticles) the influence of defects such as stacking faults and misfit dislocations is even more pronounced. Therefore, the determination of extended defects properties in these materials is of prime importance.

This study investigates the structure and energetics of extended defects in these materials by means of atomistic and electronic calculations. The simulations are performed using both quantum mechanics first-principles (or *ab initio*) calculations, and classical interatomic potentials using ridig-ions or shell model. Planar defects are investigated (through the computation of γ-surfaces) for a number of perovskite materials such as $SrTiO_3$, $PbTiO_3$, and $BaTiO_3$. The structure of dissociated dislocations in strontium titanate will also be addressed, with a comparison with experimental results and the elastic theory of dislocations.

DF 8.5 Tue 15:20 H9

Ordering in the A-site mixed perovskite $Bi_{0.5}Na_{0.5}TiO_3$ — •Melanie Gröting, Silke Hayn, and Karsten Albe — Technische Universität Darmstadt, Materialwissenschaft, Darmstadt, Germany

$Bi_{0.5}Na_{0.5}TiO_3$ (BNT) is one rare example of A-site mixed relaxor ferroelectrics. BNT-based materials show extraordinarily high strains and are thus promising environmentally friendly lead-free alternatives to the toxic standard material in piezoelectric applications $Pb(Zr,Ti)O_3$ (PZT). BNT has aliovalent cations on the A-site in the exact ratio 1:1. For B-site mixed perovskites ordering occurs when there are significant charge and size differences between the two cation species occupying the same crystallographic site. The question arises whether in A-site mixed perovskites ordering is also favored and how it would affect the materials' properties. Especially the origin of the relaxor behavior in BNT is still controversially discussed.

In order to gain insights into the ordering tendency of this material and to identify the driving forces of this process we investigated different cation configurations in 40-atoms cubic perovskite supercells by different theoretical approaches, encompassing simple ionic models and electronic density functional theory calculations. We discuss the different cation configurations with respect to their total energies, relaxation behavior and electronic properties. We find that rocksalt ordering is not the low-energy configuration if local relaxations are taken into account.

DF 8.6 Tue 15:40 H9

Temperaturabhängigkeit des Hyperfeinfeldes für ^{111}In in Al_2O_3 — •Michael Steffens[1], Reiner Vianden[1], Jakob Penner[1] und Hassan Kamleh[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nussallee 14-16, 53115 Bonn — [2]Department of physics, Faculty of sciences, University of Damascus, Syria

Der Elektronentransport in Isolatoren wird mit Hilfe der Methode der gestörten γ - γ - Winkelkorrelation (PAC) studiert. Der PAC-Sondernkern ^{111}In eignet sich für solche Untersuchungen besonders gut, da er durch Elektroneneinfang (EC) aus der eigenen Atomhülle zum ^{111}Cd zerfällt. Die dann im Cd erfolgende PAC-Messung reagiert sehr empfindlich auf die durch den EC Zerfall in der Hülle des Sondenatoms entstandene Elektronenfehlstelle und eröffnet so die Möglichkeit, das Auffüllen dieser Fehlstelle durch Elektronen aus der Gitterumgebung der Sonde zu detektieren. Der zeitliche Verlauf dieser elektronischen Relaxation, der so genannte "after effect", wird stark von der Konzentration und Beweglichkeit der Elektronen im Wirtsgitter beeinflusst, die damit auf einer Zeitskala von einigen Nanosekunden untersucht werden können.

In den Messungen an Al_2O_3-Einkristallen wurde versucht, die Verfügbarkeit der Elektronen durch Änderungen der Probentemperatur und einer dadurch erhöhten Elektronenmobilität zu steuern. Tatsächlich konnte ein Rückgang des "after effect"-Einflusses für Probentemperaturen oberhalb 800 K festgestellt werden.

Durch gezieltes Dotieren des Al_2O_3 mit Donatoren oder Akzeptoren wurde versucht die Temperatur dieses Rückganges zu beeinflussen.

DF 9: Focus Session: Structural dynamics in photoexcited molecules

Time: Wednesday 10:00–13:00 Location: H11

Invited Talk DF 9.1 Wed 10:00 H11

Structural dynamics in photoexcited molecules — •Majed Chergui — Ecole Polytechnique Fédérale de Lausanne

By combining ultrafast optical and X-ray spectroscopies, we can recover the full photocycle of molecular processes in solution. Here we will present tow examples, involving the case of ultrafast spin changes in Fe(II)-based molecular complexes, and the case of solvated halides in aqueous solutions.

5 min. break

Topical Talk DF 9.2 Wed 10:40 H11

Ultrafast reversible photogeneration of nitrosyl linkage isomers in $Na_2[Fe(CN)_5NO]2H_2O$ — •Matthieu Nicoul[1], Theo Woike[1], and Dominik Schaniel[1,2] — [1]I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany — [2]CRM2, Université de Nancy, Nancy, France

We report on the photogeneration of nitrosyl linkage isomers in single crystals of sodium nitroprusside $Na_2[Fe(CN)_5NO]2H_2O$. Using pump-probe spectroscopy with a time-resolution of 160 fs we show that the photoinduced NO rotation from a linearly bound ground state Fe-N-O to a side-on bound $\mathrm{Fe}{<}^{N}_{O}$ is completed within 1.5 ps. The relaxation after photoexcitation is mono-exponential with a time constant of 300(20) fs, indicating that during the NO rotation no intermediate state with lifetimes longer than 100 fs exists.

Topical Talk DF 9.3 Wed 11:00 H11

Photoinduced isomerization of molecular switches at metal surfaces — •Petra Tegeder — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

Molecular switches represent a fascinating class of functional molecules, whose properties can be reversibly changed between different molecular states by excitation with light or other external stimuli. Using surface science concepts like self assembly to align such molecules in a well defined geometry at solid surfaces, new functional properties may arise, which are relevant for different fields like, e.g., molecular electronics, sensing or biocompatible interfaces. For a microscopic understanding of molecular switching at surfaces, it is essential to obtain detailed knowledge on the underlying elementary processes, for instance the excitation mechanism in photoinduced switching.

I will present a case study of a specifically designed azobenzene derivative on a metal surface, namely tetra-tert-butyl-azobenzene (TBA) adsorbed on Au(111), which is so far one of the best studied system for which reversible conformational changes have been demonstrated. The trans/cis-isomerization of TBA is accompanied by reversible changes in the geometrical and electronic structure of the molecules, allowing to gain mechanistic and quantitative insight into the switching process. Our results demonstrate the feasibility of molecular switching at metal surfaces, but also indicate that the switching properties of the surface-bound species are strongly modified by the interaction with a metal substrate.

Topical Talk DF 9.4 Wed 11:20 H11
Light induced conformational changes of retinal proteins — •Heinz-Jürgen Steinhoff — Universität Osnabrück, Osnabrück, Germany

Since the discovery of the light driven proton pump bacteriorhodopsin, the scope of microbial rhodopsins has been considerably extended in view of their functional properties as pumps, sensors, and channels. The structures of these membrane proteins are related, and, as we have shown by electron paramagnetic resonance (EPR) spectroscopy in combination with site-directed spin labeling, light induced isomerisation of the retinal chromophore initiates similar conformational changes in the protein scaffold of bacteriorhopodsin and sensory rhodopsin SRII. The light receptor SRII, in complex with the receptor specific transducer, HtrII, is responsible for the negative phototaxis of halobacteria. The talk focuses on time resolved EPR detection of light induced conformational changes of SRII, which reveals unique conformational rearrangements and uncovers the mechanism of the signal transfer from SRII to the associated transducer HtrII.

Invited Talk DF 9.5 Wed 11:40 H11
Ultrafast photochromism of fulgides — •Markus Braun[1,2], Simone Draxler[2], Thomas Brust[2], and Stephan Malkmus[2] — [1]Institut für Physikalische und Theoretische Chemie, Johann Wolfgang Goethe-Universität Frankfurt, Max von Laue-Strasse 7, 60438 Frankfurt am Main, Germany — [2]Lehrstuhl für BioMolekulare Optik, Oettingenstr. 67, Ludwig-Maximilians-Universität München, 80538 München, Germany

Pump-probe spectroscopy with fs-time resolution is a powerful tool to elucidate reaction pathways of complex photoreactions. We use pulse sequences to trigger and influence the reaction dynamics of photochromic indolylfulgides [1]. These experiments give deeper insight in the mechanism of the light-induced pericyclic ring-opening/ring-closure reactions for those molecular switches. The pericyclic reactions occur ultrafast without long-lived intermediates and are associated with a definite change of the steady state absorption spectrum. The ground state isomers are thermally stable, which is favourable for distinct applications (memory) [2]. The ultrafast photoreactions are studied by fs-pump-probe spectroscopy in the UV/Vis and the influence of vibrational excess energy (temperature, wavelength, pre-excitation) on the dynamics and yield is investigated [3].

[1] S. Draxler et al., Phys. Chem. Chem. Phys. 11 (2009) 5019-5027
[2] S. Malkmus et al., Adv. Funct. Mater. 17 (2007) 3657-3662
[3] T. Brust et al., J. Photochem. Photobiol. A 207 (2009) 209-216

5 min. break

Topical Talk DF 9.6 Wed 12:20 H11
***Ab-initio* and semi-empirical molecular dynamics studies of photo-isomerisable molecules** — •Jan Boyke Schönborn, Ole Carstensen, and Bernd Hartke — Christian-Albrechts-University Kiel, Germany

Due to the ongoing trend to miniaturization the interest in molecular scale switches is growing fastly. Fulgides and Azobenzenes are promising systems for future applications. The talk is going to present recent theoretical results on the photochemical properties and dynamics of derivatives of the aforementioned molecules. After careful evaluation by comparison to high level *ab-initio* data (CASSCF/CASPT2), different semi-empirical multireference methods have been used in *ab-initio* molecular dynamics simulations to get a deepened understanding of the ultrafast switching processes. Transient spectra covering a wavelength range of 500 nm and a time period of 1500 fs have been simulated, including 3-5 electronically excited states. The excellent agreement of these simulated spectra with the experimental ones allows for a confident interpretation in terms of mechanistic details. An in-depth analysis of the calculated trajectories indicates that even seemingly minor modifications of the functional groups play major roles in the control of the switching dynamics. Possible ways of simulating switchable molecules embedded in bulk soft matter are discussed briefly.

Topical Talk DF 9.7 Wed 12:40 H11
Influence of ligand substitution and dielectric environment on structural dynamics in photoswitchable molecular compounds — •Volker Dieckmann, Sebastian Eicke, Kristin Springfeld, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Tuning of photoswitchable molecular compounds by ligand substitution or alteration of the dielectric environment is motivated either to reveal deeper physical insight to the underlying molecular switching mechanisms or the targeted molecular design in various applications such as in biomimetics. In this talk, we highlight our results on: (a) ligand substitution at the example of $[\mathrm{Ru(bpy)_2(R\text{-}OSO)}]^+$ solved in propylene carbonate with different ligands R; (b) an altered dielectric environment at sodium nitroprusside compounds electrostatically attached to TiO_2 thin films in comparison to a liquid solution. The impact of these alterations is studied optically by means of time-resolved absorption spectroscopy in the VIS and IR-spectral range, which is related to structural changes upon light-exposure via changes in the molecular polarizability and molecular vibrations. While only slight changes are verified by ligand substitution in the sulfoxide compounds, the photofunctionality of the nitrosyl compound changes dramatically from light-induced linkage isomerization into a photo-release of the NO-bond.

Financial support by the DFG (project GRK 695) is gratefully acknowledged.

DF 10: Dielectric surfaces and interfaces

Time: Wednesday 14:00–17:30 Location: H11

Invited Talk DF 10.1 Wed 14:00 H11
Molecular self-assembly on calcite — •Angelika Kühnle, Philipp Rahe, Jens Schütte, and Sebastian Rode — Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, 55099 Mainz

Calcite, the most stable polymorph of $CaCO_3$, is one of the most abundant minerals on earth that plays a crucial role in a variety of different fields such as biomineralization and environmental geochemistry. Moreover, calcite precipitates upon scaling, a process that is deliberately prevented by polyelectrolyte addition in many daily life as well as industrial applications such as laundry and water desalination.

Consequently, the $(10\bar{1}4)$ calcite cleavage plane as well as molecule adsorption onto calcite $(10\bar{1}4)$ has attracted great attention. Despite this, a controversy exists as to whether the $(10\bar{1}4)$ cleavage plane of calcite reconstructs or not. Atomically resolved scanning force microscopy images taken in liquids will be presented, revealing a bulk-truncated (1x1) surface. When imaged under ultra-high vacuum conditions, however, clear experimental evidence is provided for a (2x1) reconstruction.

Self-assembly of different functionalized organic molecules on calcite will be reported, demonstrating the formation of both, twodimensional ordered molecular layers as well as uni-directional wire-like structures.

5 min. break

DF 10.2 Wed 14:45 H11

Room temperature domain wall conductivity in Mg-doped lithium niobate — •Mathias Schröder, Alexander Haussmann, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Deposition routes for metallic and molecular nanowires on the 180° domain walls of lithium niobate through ferroelectric lithography are well established [1,2]. However, a detailed understanding of the underlying processes is still missing, which implies the necessity of further systematic studies of specific domain wall properties.

Here, we report on conductive-AFM (c-AFM) measurements on 5 mol% Mg-doped congruent $LiNbO_3$ single crystals. We compare the c-AFM results with the domain distribution recorded by piezoresponse force microscopy (PFM). Surprisingly, we find an enhanced current density at room temperature and in air along the 180° domain walls under UV-illumination above the band gap of 4 eV. This domain wall conductivity was then studied as a function of wavelength and light intensity. Implications for ferroelectric lithography on $LiNbO_3$ templates will be discussed.

[1] S.V. Kalinin et al., *Nano Letters* **2**, 589 (2002).

[2] A. Haussmann et al., *Nano Letters* **9**, 763 (2009).

DF 10.3 Wed 15:05 H11

Theoretical atomic-scale study of the interaction of grain boundaries with domain walls in ferroelectric $PbTiO_3$ — •Pavel Marton and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Perovskite-type ferroelectric ceramics for actuators and sensors like $PbTiO_3$ or $Pb(Zr,Ti)O_3$ have dense polycrystalline microstructures. Within micrometer-sized grains, even smaller ferroelectric domain structures are found. Both domain walls (DW) and grain boundaries (GB) play an important role in the macroscopic material performance.

An objective of this work is an investigation of fundamental properties of interactions of DW with GB in tetragonal $PbTiO_3$. Atomic-scale experimental observations of GB in perovskites are rare and difficult to obtain. Therefore, the interfaces studied theoretically in this work were motivated by experimental observations of Sigma=3 [1] and Sigma=5 [2] symmetrical tilt GB in $SrTiO_3$. We focus on interfaces, which are both GB and ferroelectric DW. Atomic structures were obtained using atomistic shell-model simulations and ab-initio density functional theory (DFT) calculations. For the chosen GB, DFT calculations provide detailed insight into atomic arrangements, energetic stabilities and electronic states of the interfaces. We discuss properties of GB with DW in dependence on their type, and we compare them with properties of interfaces in cubic $SrTiO_3$ [3].

[1] S. Hutt et al., J. Phys.: Condens. Matter 13 3949 (2001).

[2] M. Imaeda et al., Phys. Rev. B 78 245320 (2008).

[3] N. Benedek et al., Phys. Rev. B 78, 064110 (2008).

DF 10.4 Wed 15:25 H11

An electronic defect state analysis in perovskite heterostructures by surface photovoltage spectroscopy — •Jana Becherer, Elke Beyreuther, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Surface photovoltage (SPV) spectroscopy provides a nondestructive, contact-free method to characterize and quantify electronic trap states within the bandgap of a semiconducting material. In the present study we apply the method to determine electronic defect states of wide-bandgap perovskite oxides.

For different perovskites ($SrTiO_3$ and $BaTiO_3$ single crystals, lead zirconate titanate and lanthanum manganite thin films on $SrTiO_3$ substrates) wavelength-, intensity-, temperature-, and time-resolved surface photovoltage spectroscopy was performed using a Kelvin probe setup in air. Analysis of these measurements provides surface, interface, and bulk state properties, i.e., their energy position and distribution, density, and transition probabilities such as the thermal and optical cross sections. We discuss the results and their impacts in detail.

DF 10.5 Wed 15:45 H11

In situ high pressure synchrotron photoemission study of the $SrTiO_3$/Pt interface — •Robert Schafranek[1], Christoph Körber[1], Andre Wachau[1], Andreas Klein[1], Michael Haväcker[2], Axel Knop-Gericke[2], and Robert Schlögl[2] — [1]Darmstadt University of Technology, Institute of Materials Science, Surface Science Division, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Fritz-Haber Institute, Department of Inorganic Chemistry, Faradayweg 4-6, 14195 Berlin, Germany

The $(Ba,Sr)TiO_3$/Pt interface present e.g. in tunable capacitors for microwave applications plays a crucial role for device properties, which can be explained by a variation of the Schottky barrier height with preparation conditions. It has been shown by photoemission experiments that the barrier height can be reversibly switched between a reduced state with a low barrier height (0.5 eV) and an oxidized state with a high barrier height (>1.2 eV) by annealing at 400°C in vacuum and oxygen, respectively. An in situ high pressure synchrotron photoemission study of the $SrTiO_3$/Pt interface was carried out for further understanding of the dependence of the Schottky barrier height on the O_2 pressure. The experiments were performed at the ISISS dipole beamline at the BESSY II synchrotron in Berlin at different temperatures using a $SrTiO_3$:Nb single crystal covered with a 3 nm thick Pt layer. A modification of the barrier height of 1eV could be observed even for the lowest used sample temperature of 100 °C. Furthermore the variation of the barrier height with O2 pressure could be verified by O2 pressure-dependent I-V measurements.

5 min. break

DF 10.6 Wed 16:10 H11

$(Ba,Sr)TiO_3$ tunable capacitors with Al_2O_3 barrier layer — •Shunyi Li[1], Yuliang Zheng[2], Andre Wachau[1], Robert Schafranek[1], Rolf Jakoby[2], and Andreas Klein[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Mikrowellentechnik, Technische Universität Darmstadt, Darmstadt, Germany

$(Ba,Sr)TiO_3$, due to its high non-linearity of dielectric constants under electric field, is considered as a promising material for tunable integrated components for microwave applications. However, the high dielectric loss and high leakage current still remain a main impediment, where the interface between electrodes and dielectrics plays an important role. BST varactors with Al_2O_3 barrier layers at the interfaces are prepared via RF magnetron sputtering. The interface formation has been studied by using x-ray photoelectron spectroscopy with in situ sample preparation. A high energy barrier for electrons is formed at the BST/Al_2O_3 contact. Leakage current measurements show that the injection of charge carriers into dielectrics can be effectively reduced by the barrier layer. Significant changes of dielectric properties are observed during dielectric characterizations. The capacitance and the tunability are reduced due to the insertion of Al_2O_3, and the overall capacitance can be well simulated by serial capacitor model. The quality factor of the varactor is improved due to the better insulating interfaces. By introducing the Al_2O_3 layer, charged interfaces are observed in the dielectric measurements, which is considered as the result of accumulation of charge carriers at the BST/Al_2O_3 interfaces.

DF 10.7 Wed 16:30 H11

Energy level alignment and electric and dielectric properties of BST with ITO electrodes — Shunyi Li, •Cosmina Ghinea, André Wachau, Robert Schafranek, and Andreas Klein — Petersenstraße 23, 64287 Darmstadt, Germany

The interface formation of (Ba, Sr) TiO3 thin films and magnetron sputtering SrTiO3 single crystal with transparent conducting Sn-doped indium oxide (ITO) have been studied by photoelectron spectroscopy with in situ sample preparation via RF. The energy level alignment indicates a very small barrier height at the ITO / BST and STO / ITO interfaces. Current-voltage and dielectric measurements have been performed on BST thin films with parallel-plate structure using Pt and ITO for both top and bottom electrodes. A strong influence of electrode materials on electrical and dielectric properties of the BST films is observed. BST capacitors with Pt electrodes show a back-to-back diode behavior and a relatively low leakage current and high dielectric constant. In contrast, the BST films with ITO electrodes show high leakage currents and high dielectric losses.

DF 10.8 Wed 16:50 H11

Energy band alignment between $Pb(Zr,Ti)O_3$ and high and

low work function conducting oxides - from hole to electron injection — •Robert Schafranek[1], Feng Chen[1], Shunyi Li[1], Wenbi Wu[2], and Andreas Klein[1] — [1]Darmstadt University of Technology, Institute of Materials Science, Surface Science Division, Petersenstrasse 23, D-64287 Darmstadt, Germany — [2]Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, People's Republic of China

Metal/oxide interfaces are important for a variety of applications. For example in ferroelectric random access memories based on $Pb(Zr,Ti)O_3$ (PZT) the fatigue (reduction of the of the polarization with switching cycles) depends substantially on the used electrode material. While for Pt electrodes a fast degradation of the polarization is reported, this effect is not observed for RuO_2 electrodes up to 1012 cycles. The contact properties between $Pb(Zr,Ti)O_3$ and the high work function conducting oxide RuO_2 respectively the low work function conducting oxide In_2O_3:Sn (ITO) were studied using in situ photoelectron spectroscopy (PES). In an ultra high vacuum system stepwise deposition of RuO_2 and ITO on PZT thin films by magnetron sputtering and interface characterization via PES were carried out without breaking vacuum. From the PES experiments a smaller barrier for the hole injection into PZT is found for RuO_2 while for ITO the injection of electrons is favored.

DF 10.9 Wed 17:10 H11

Preparation and dielectric investigation of organic metal insulator semiconductor (MIS) structures with a ferroelectric polymer — René Kalbitz[1], Peter Frübing[1], Reimund Gerhard[1], and •Martin Taylor[2] — [1]Department of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476, Potsdam, Germany — [2]School of Electronic Engineering, Bangor University, Dean Street, Bangor Gwynedd, LL57 1UT, UK

Ferroelectric field effect transistors (FeFETs) offer the prospect of an organic-based memory device. Since the charge transport in the semiconductor is confined to the interface region between the insulator and the semiconductor, the focus of the present study was on the investigation of this region in metal-insulator-semiconductor (MIS) capacitors using dielectric spectroscopy. Capacitance-Voltage (C-V) measurements at different frequencies as well as capacitance-frequency (C-f) measurements after applying different poling voltages were carried out. The C-V measurements yielded information about the frequency dependence of the depletion layer width as well as the number of charges stored at the semiconductor/ insulator interface. The results are compared to numerical calculations based on a model introduced by S. L. Miller (JAP, 72(12), 1992). The C-f measurements revealed three main relaxation processes. An equivalent circuit has been developed to model the frequency response of the MIS capacitor. With this model the origin of the three relaxations may be deduced.

DF 11: High-k and Low-k Dielectrics I (Joint Session DS/DF)

Time: Wednesday 9:30–11:00 Location: H8

DF 11.1 Wed 9:30 H8

Spectroscopic investigations of interaction between C_{60} fullerene and nitrogen atom from amine group — •Jolanta Klocek[1], Daniel Friedrich[1], Kostyantyn Zagorodniy[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany — [2]Institute for Solid State and Materials Research, IFW Dresden, PF 270116, D-01171 Dresden, Germany

We investigated interactions between fullerene molecule and amine group from 3-aminopropyl-trimethoxysilane (3AT). Theoretical calculations show that the material obtained as a result of interactions between 3AT and C_{60} fullerene may have extremely low dielectric constant around 1.6, so it could be considered as a candidate for ultra low-k (ULK) material applications. We prepared films composed of 3AT and fullerene by using two preparation techniques: spin-coating and evaporation. Interactions between these two components were investigated by using X- ray photoelectron spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS). We found that there are strong chemical reactions between the nucleophilic nitrogen atom from 3AT and electrophilic fullerene molecule. Results of NEXAFS measurements suggest that due to direct interactions between 3AT and C_{60} the shape of fullerene molecule is changed.

DF 11.2 Wed 9:45 H8

The influence of elastic and inelastic processes on trap assisted tunnelling through thin dielectric films — •Grzegorz Kozlowski, Jarek Dabrowski, Piotr Dudek, Gunther Lippert, and Grzegorz Lupina — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) , Germany

Impurities or structural imperfections of the crystal may introduce discrete electronic states (or a band when defects interact with one another) into the band gap of the dielectric. Electrically active defects can be used in a trap assisted tunnelling (TAT) process giving a noticeable contribution to the leakage and to the total current.

We developed a simple quantum mechanical model to investigate the role of defects in leakage current through thin dielectric films for future DRAM applications. The influence of image force as well as a possible charge state of an empty trap was considered. The results of numerical simulation were used to characterize the electrical behaviour of thin dielectric films at different temperatures. The temperature dependence may come from two phenomena. The first one is the Boltzmann distribution of charge carriers in the electrodes. In a limited way one can reproduce the temperature dependence of the leakage by considering various distribution of defects in energy and position in the film. This approach is however insufficient to reproduce the dependence in the whole regime of applied voltages. We thus expanded our model by including an additional type of process, i.e. the electron-phonon coupling which gave rise to non-radiative multiphonon processes.

DF 11.3 Wed 10:00 H8

Electrically optimized high-κ metal gate MOSFET by specific modification of the band alignment — •Łukasz Starzyk, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, Cottbus D-03046, Germany

The electrical optimization of metal/oxide/semiconductor gate stacks by specific modification of the band alignment for advanced MOS technology incorporating high dielectric constant (κ) materials is explored. Because of requirements concerning continued scaling of MOSFET transistors, gate oxides and cobalt electrode have been grown successively on Si substrate respectively by means of atomic layer deposition (ALD) and evaporation. The thicknesses of high-κ films were around 2 nm. In case of work function engineering, interfaces' chemistry plays a fundamental role. We applied synchrotron radiation based x-ray photoelectron spectroscopy (SR XPS) to characterize our samples, which allows step by step *in situ* investigations. Co 2p, Al 2p, Hf 4f, Si 2p and O 1s core levels spectra were measured and analyzed. From valence band (VB) spectra we determined Schottky barrier height and electronic bands offsets.

DF 11.4 Wed 10:15 H8

A comparison of $(SrO)_x(ZrO_2)_{(1-x)}$ and ZrO_2 as potential high-k dielectric for future memory applications — •Matthias Grube[1], Dominik Martin[1], Walter Michael Weber[1], Thomas Mikolajick[1], Lutz Geelhaar[2], and Henning Riechert[2] — [1]Namlab GmbH, 01187 Dresden — [2]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

Following the demands of the aggressive downscaling of the capacitor area of dynamic random access memories, a material screening of novel high-k dielectrics with nanometer-scale thicknesses is required. Pure ZrO_2 and admixtures with SrO are promising examples as possible substitutes for the established materials. Their growth, their physical and electrical characterization is our contribution to the screening. We employed molecular beam deposition to grow thin layers of $(SrO)_x(ZrO_2)_{(1-x)}$ on n^{++}-Si substrates with a predeposited 5nm thin TiN layer as bottom electrode to realize metal-insulator-metal structures. An extensive physical characterisation consisting of X-ray diffraction, X-ray fluorescence analysis, X-ray reflectometry and atomic force microscopy was performed to verify the crystallinity, the stoichiometry, the physical thickness and the surface morphology of the dielectric film itself. The interface between the dielectric and the bottom electrode was investigated by transition electron microscopy. I-V and C-V measurements revealed k-values consistent to the literature for ZrO_2. However, for $(SrO)_x(ZrO_2)_{(1-x)}$ rather low k-values below 9 for films up to 20 nm and much higher k-values of about 50 for films of 40 nm thickness were observed. Those dependencies will be discussed.

DF 11.5 Wed 10:30 H8

Nanoscale analysis of the electric properties of ultra thin ZrO_2-, $(ZrO_2)_x(Al_2O_3)_{1-x}$- and $ZrO_2/Al_2O_3/ZrO_2$-films. — •Dominik Martin[1], Matthias Grube[1], Elke Erben[1], Wenke Weinreich[2], Uwe Schröder[1], Lutz Geelhaar[3], Walter Weber[1], Henning Riechert[3], and Thomas Mikolajick[1] — [1]namlab Gmbh, D-01187 Dresden — [2]Fraunhofer-CNT, D-01099 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin

In order to achieve an high k-value in sub 10 nm thin films of ZrO_2 it is necessary to reach the tetragonal crystalline phase. This is done by either depositing the layer at higher temperatures or by a post deposition annealing step. Both however induce high leakage current through the layer. Small amounts of Al_2O_3 can be incorporated in ZrO_2 to reduce leakage current. In order to understand the detailed charge carrier transport mechanisms, thickness series of ultra thin ZrO_2-, $(ZrO_2)_x(Al_2O_3)_{1-x}$- and $ZrO_2/Al_2O_3/ZrO_2$-films were deposited by Atomic Layer Deposition and subjected to different rapid thermal annealing processes. These layers were examined by I-V-, C-V-Spectroscopy and conductive atomic force microscopy. It is shown that Al incorporation throughout the entire layer imposes the relatively low k value of Al_2O_3 onto the entire layer. Whereas incorporation of only to cycles of Al into the center of the ZrO_2 effectively reduces leakage currents while maintaining a higher k value.

DF 11.6 Wed 10:45 H8

Atomic Vapour Deposition of TiTaO for MIM applications — •Mindaugas Lukosius[1], Canan Baristiran Kaynak[1], Christian Wenger[1], Günther Ruhl[2], and Simon Rushworth[3] — [1]IHP, Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]Infineon, Wernerwerkstr. 2, 93049 Regensburg, Germany — [3]SAFC HiTech, Bromborough, Wirral, Merseyside, U.K. CH62 3QF

Metal-Insulator-Metal (MIM) capacitors are widely used in ICs for Radio-Frequency (RF) applications. Currently, capacitors fabricated by performing MIM structures use silicon oxide or silicon nitride as an insulating layer. However, the capacitance density of these materials is limited by low dielectric constant values. Therefore, for further integration of passive components such as capacitors into CMOS devices, dielectric materials with higher permittivity than SiO2 (k = 3.8) are required. Atomic Vapor Deposition (AVD*) technique was successfully applied for the first time for depositions of TiTaO oxide films on 8-inch wafers using two separate Ti(OPri)2(mmp)2 and TBTDET precursors for MIM applications in back-end of line (BEOL). Composition, crystalinity and electrical properties such as dielectric constant, capacitance and leakage currents were studied in Au/TiTaO/TiN/Si MIM capacitors. The effect of post deposition annealing (PDA) and investigation of different top electrode materials will be also presented.

DF 12: High-k and Low-k Dielectrics II (Joint Session DS/DF)

Time: Wednesday 11:15–12:45 Location: H8

DF 12.1 Wed 11:15 H8

Electrical and structural characteristics of SrTaO/SrTiO based M-I-M capacitors — •Canan Baristiran Kaynak[1], Mindaugas Lukosius[1], Bernd Tillack[1], Christian Wenger[1], Guenther Ruhl[2], and Tom Blomberg[3] — [1]IHP Im Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]Infineon Technologies AG, Wernerwerkstr. 2, 93049 Regensburg, Germany — [3]ASM Microchemistry Ltd., Väinö Auerin katu 12 A, 00560 Helsinki, Finland

In this work, on-chip M-I-M capacitors are realized using SrTiO /SrTaO dielectric stacks. The deposition of the SrTiO dielectric is done by ALD and to get a crystalline state correspondingly high k value, 550 °C annealing temperature is applied. Moreover, SrTaO is considered as a part of barrier stack due to its amorphous characteristic at 550°C annealing temperatures. In this way, it is expected to improve the electrical characteristic of the devices. A set of M-I-M stacks such as Au/SrTiO/TaN/Si, Au/SrTaO/SrTiO/TaN/Si and Au/SrTiO/SrTaO/TaN/Si have been deposited and analyzed by means of electrical and analytical characterizations. The effect of thickness of SrTaO was also evaluated. From the C-V and J-V measurements, dielectric constant, corresponding capacitance densities and leakage current performance were extracted. For the investigation of interfaces between the stacks XPS and ToF-SIMS were utilized. The results mainly demonstrate that the use of SrTaO material in the barrier stack strongly improves the leakage current density of M-I-M capacitors due to its amorphous state which serves as a strong barrier between the dielectric and the electrode of the M-I-M capacitor.

DF 12.2 Wed 11:30 H8

Resistive switching in $TiN/HfO_2/Ti/TiN$ MIM structures for future memory applications — •Christian Walczyk[1], Christian Wenger[1], Mindaugas Lukosius[1], Mirko Fraschke[1], Ioan Costina[1], Sebastian Schulze[1], Sebastian Thiess[2], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — [2]Hasylab at DESY, Notkestrasse 85, 22607 Hamburg, Germany.

The electrically switchable resistance change phenomenon between a high (OFF-state) and a low (ON-state) resistive state of a metal-insulator-metal (MIM) diode structure has attracted considerable attention in recent years for future non-volatile memory applications (RRAM). Especially hafnium dioxide (HfO_2) as insulator is among the oxides particularly desirable due to the fact that it is nowadays considered as a BEOL Si CMOS compatible binary metal oxide system. Typical bipolar current-voltage characteristics of a $TiN/HfO_2/Ti/TiN$ stack with a HfO_2 thickness of 10 nm will be presented. The switching properties crucially depend on a) whether the additional Ti layer is integrated as top or bottom electrode and b) on the application of post-deposition annealings (PDA). To unveil the origin of these observations, a materials science study by TOF-SIMS, TEM and HA-XPS was carried out. It is possible to prove that this metallic Ti layer getters during the PDA treatments oxygen from HfO_2, resulting in the formation of non-stoichiometric HfO_x. Due to their significance in NVM technology, we will furthermore present the retention and cycling endurance characteristics.

DF 12.3 Wed 11:45 H8

Oxygen Engineering of HfO_{2-x} Thin Films grown by Reactive Molecular Beam Epitaxy — •Erwin Hildebrandt[1], Jose Kurian[1], Peter Zaumseil[2], Thomas Schröder[2], and Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU-Darmstadt — [2]IHP, Frankfurt, Oder

Reactive Molecular Beam Epitaxy (R-MBE) is an ideal tool for tailoring physical properties of thin films to specific needs. For the development of cutting-edge oxides for thin film applications a precise control of oxygen defects is crucial. R-MBE in combination with rf-activated oxygen allows reproducibly growing oxide thin films with precise oxidation conditions enabling oxygen engineering.

R-MBE was used to grow Hf and $HfO_{2\pm x}$ thin films with different oxidation conditions on sapphire single crystal substrates. Structural characterization was carried out using rotating anode x-ray diffraction revealing highly textured to epitaxial thin films on *c*-cut sapphire. Furthermore, switching of film orientation by varying the oxidation conditions was observed demonstrating the role of oxygen in the growth procedure. The investigation of electrical properties using a four probe measurement setup showed conductivities in the range of 1000 $\mu\Omega$cm for oxygen deficient HfO_{2-x} thin films. Optical properties were investigated using a photospectrometer and additionally x-ray photoelectron spectroscopy was carried out to study the band gap and valence states. Both techniques were used to monitor the oxygen content in deficient HfO_{2-x} thin films. Our results demonstrate the importance of oxygen engineering even in the case of 'simple' oxides.

DF 12.4 Wed 12:00 H8

Band structure and electrical properties of MBE grown HfO_2

- based alkaline earth perovskites — •Dudek Peter[1], Łupina Grzegorz[1], Kozłowski Grzegorz[1], Dabrowski Jarek[1], Lippert Gunther[1], Müssig Hans-Joachim[1], Schmeisser Dieter[2], and Schroeder Thomas[1] — [1]IHP-Microelectronics, Im Technologiepark 25, D-15236 Frankfurt (Oder) — [2]BTU Cottbus, Konrad-Wachsmann-Allee 17, D-03046 Cottbus, Germany

Ultra thin dielectric films ($<$20 nm) deposited on TiN electrodes are interesting for MIM capacitor application. High capacitance density and dielectric permittivity must be accompanied by extremely low leakage currents (10^{-8} A/cm^2) at bias 0.5 V. To achieve such low leakage currents, high band gap and proper band alignment is required. Occupied electronic states can be probed with standard laboratory photoemission methods. Probing of unoccupied states is more challenging. Synchrotron based PES in combination with XAS forms a powerful method to study the band alignment. ASAM end station located at the U 49/2 PGM 2 beamline of BESSY II (Berlin) offers excellent conditions for performing such measurements. We investigated HfO_2 - based alkaline earth perovskite - $BaHfO_3$ with subsequent admixture of TiO_2, resulting in formation of $BaHf_{0.5}Ti_{0.5}O_3$ compound. The analysis of data indicates that band gap for HfO_2 is similar to $BaHfO_3$ and amounts 5.8 eV; for $BaHf_{0.5}Ti_{0.5}O_3$ it decreases to 3.8 eV. We conclude that the addition of TiO_2 to $BaHfO_3$ increases significantly the dielectric permittivity but also impacts the band gap alignment. The conduction band offset shrinks, influencing the leakage current behavior.

DF 12.5 Wed 12:15 H8

In-situ EELS and UPS measurements on HfO_2 ALD layers — •Marcel Michling, Massimo Tallarida, Krzysztof Kolanek, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, K.-Wachsmann-Allee 1, 03046 Cottbus

In this contribution we report on our in-situ cycle-by-cycle (up to 10 cycles) investigations of the HfO_2 ALD process using the methods of EELS and UPS.

We used TDMA-Hf as a precursor and p-type Si wafer with natural oxide as the substrate. The EELS measurements were done with a primary energy of 52,5 eV and the UPS measurements with He I (21,218 eV).

The change in the onset of the loss function is readily observed. Already after two cycles the value approach to the bulk value of HfO_2. Upon ALD growth there is a remarkable decrease in the intensity of states within the gap. They are rather smooth and saturate after 10 cycles. With UPS we follow the variation of the VB onset and changes in the secondary electron onset. We summarize our data in a band diagram not based on bulk values but on cycle dependent quantities. With these cycle-by-cycle experiments we study the initial growth of HfO_2 especially in the very first cycles.

DF 12.6 Wed 12:30 H8

Determination of interfacial layers in high - k ALD nanolaminate materials by ARXPS and SRXPS measurements. — •Jakub Wyrodek[1], Massimo Tallarida[1], Dieter Schmeisser[1], and Martin Weisheit[2] — [1]Brandenburgische Technische Universität, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, Cottbus D-03046, Germany
— [2]GLOBALFOUNDRIES, Dresden, Germany

The interfacial layers of high dielectric constant (high - k) nanolaminate films are here explored. Problems concerning ALD nanolaminate layers deals mainly with lack of accurate methods to determine in depth profile of few nm thick stacks. Modified angle resolved XPS(ARXPS) and synchrotron radiation XPS(SRXPS) are proposed as methods suitable in layer profiling. Studied stacks containing ZrO/HfO or AlO/ZrO, were prepared on Si substrates by atomic layer deposition (ALD). Two sets of experiments were covered. First dealt with initial growth (up to 20 cycles, with thickness d $<$ 2nm) of AlO/ZrO and included layer by layer *insitu* investigation by SRXPS. Second experiment refer to industrial grown ZrO/HfO films (d $\sim$ 3nm) processed with various parameters resulting in both, layer by layer and homogenous depositions. For those samples *exsitu* XPS, with angle dependent variation of probing depth, measurements were covered. By comparing obtained intensity ratios for different angles with computational developed stack model it was found that no simple layer by layer but some intermixing growth occurred including interaction with silicon substrate.

DF 13: Poster II: Electrical, mechanical and optical properties, nonlinear dielectrics

Time: Wednesday 15:00–17:30 Location: Poster A

DF 13.1 Wed 15:00 Poster A

Barrier heights, polarization switching and electrical fatigue in PZT ceramics with different electrodes — •Andreas Klein, Jürgen Rödel, Heinz von Seggern, Torsten Granzow, Feng Chen, Sergey Zukov, Robert Schafranek, Andre Wachau, and Julia Glaum — Technische Universität Darmstadt, Institute of Material Science, Petersenstraße 32, D-64287 Darmstadt, Germany

Metal Pt, transparent conductive oxide ITO (In_2O_3:10at% Sn) and metal oxide RuO_2 were deposited by sputtering on PZT ceramics as electrodes. The Schottky barrier heights at the ferroelectric/electrode interfaces are determined by photoelectron spectroscopy. The barrier heights vary significantly and indicate a preference for either hole or electron injection. The polarization, strain, permittivity, and piezoelectric constant hysteresis loops are, however, identical for all electrodes. Very small changes are observed in the polarization dependence on time and applied field, which was studied over a broad time window ranging from 10^{-7} to 10^2 s for applied fields between 1 and 2 kV/mm. A 20% reduction of polarization after 10^6 bipolar cycling is observed for all the samples. In contrast to PZT thin films, the loss of remanent polarization with bipolar switching cycles does not depend on electrode material, indicating a different fatigue mechanism for thin film and bulk ceramics.

DF 13.2 Wed 15:00 Poster A

Low frequency properties of space-charge wave excitation — •Thomas Schemme, Burkhard Hilling, Kay-Michael Voit, Heinz-Jürgen Schmidt, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

One possibility for the excitation of space-charge waves (SCW) in semi-insulating materials is the illumination with a superposition of one static and one moving interference pattern with equal spatial frequency and the application of a static electric field [1]. In this case, a constant ac signal at frequencies lower the resonance frequency of the SCW is uncovered. This low frequency signal does not persist using an oscillating pattern for excitation, i.e., it is a particular artefact of the four-beam excitation. To analyze this additional signal, both methods are analyzed comparatively in terms of their light pattern. We discuss the origin of the low frequency signal in the frame of a spatial modulation of the photoconductivity and give experimental evidence for our model approach. Thereby, a brief introduction into the theory describing the SCW-signal is presented. Financial support from the Deutsche Forschungsgemeinschaft within the Graduate College 695 is gratefully acknowledged.

[1] B. Hilling *et al.*, PRB **80**, 205118 (2009)

DF 13.3 Wed 15:00 Poster A

Light-induced linkage isomerization of photochromic $[\mathrm{Ru(bpy)_2(R\text{-}OSO))}]^+$ compounds — •Kristin Springfeld[1], Volker Dieckmann[1], Sebastian Eicke[1], Mirco Imlau[1], and Jeffrey J. Rack[2] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]Department of Chemistry and Biochemistry, Ohio University, Athens, Ohio 45701

Ruthenium sulfoxides exhibit light-induced linkage isomerization of the SO-bond with remarkable photosensitivity $S = (0.25 \pm 0.03)\,\mathrm{Ws\,cm^{-1}}$ and extended lifetimes of the related metastable states in the order of 10^4 s [1]. The isomerization is accompanied with tremendeous changes of the optical extinction up to $9350\,\mathrm{cm^{-1}\,mol^{-1}}$ thus enabling the study of linkage isomerization by means of time-resolved optical spectroscopy. Here, the influence of ligand substitution is studied via inspection of the photosensitivity and the generation and relaxation dynamics of the photochromic response as a function of temperature (pump at $\lambda = 405$ nm , probe at $\lambda = 532$ nm). The spectra of the modified compounds, where ligands R = Bn, BnCl, and BnMe were attached to OSO, were compared with the reference system $[\mathrm{Ru(bpy)_2(OSO)}]^+$. It turns out, that the new ligands affect the absorption features and the photosensitivity of the system only slightly. In contrast, a strong influence of the thermal relaxation of the metastable states is uncovered. Remarkably, the influence on the frequency factors is much more pronounced than on the activation energies achieved by Arrhenius' law.

[1] Dieckmann et al., Opt. Express, 17, 15052 (2009)

DF 13.4 Wed 15:00 Poster A

Phototriggered NO and CN release from $[\mathrm{Fe(CN)_5NO}]^{2-}$ molecular monolayers attached to $\mathrm{TiO_2}$ surfaces — •Volker Dieckmann[1], Mirco Imlau[1], Dereje Hailu Taffa[2], Lorenz Walder[2], Robert Lepski[3], Dominik Schaniel[3], and Theo Woike[3] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]Institute of Chemistry, Universtity of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [3]I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Phototriggered NO and CN release from $[\mathrm{Fe(CN)_5NO}]^{2-}$ (NP) molecular monolayers is studied by a combination of electrochemistry, infrared spectroscopy, and mass spectrometry under light exposure at temperatures of 80 K and 294 K. The NP molecular monolayers were electrostatically attached to thin films of mesoporous $\mathrm{TiO_2}$ deposited on silicon. Irradiation of the surfaces results in NO and CN release, which is verified with mass spectrometry. The kinetics of the NO release are determined by inspection of the ν_{NO} stretching mode as a function of exposure to light in the violet/green spectral range. The decrease of the ν_{NO}-amplitude can be modeled considering the NO release as a two-step process with an intermediate state between the attached and the released state. According to literature, the intermediate state may be related to the light-induced linkage NO isomerization of the NP. Financial support by the DFG (GRK 695, WO618/8-1), the federal state of Lower Saxony (Lichtenberg-Stipendium) and the BMBF (FKZ 03X5510) is gratefully acknowledged.

DF 13.5 Wed 15:00 Poster A

Time-resolved analysis of short-living mixed phase and amplitude gratings — •Raphael-Sung Hardt, Hauke Bruening, Bettina Schoke, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The time-resolved analysis of short-living mixed phase and amplitude gratings is a demanding challenge in materials with an optical response originating from optically excited, metastable states. For instance, such gratings appear in materials featuring the optical generation of strongly localized charge carriers or photo-induced linkage isomerism in molecular crystals. An established tool for volume grating analysis is the determination of the diffraction efficiency as a function of the angular detuning $\Delta\theta_B$ from the Bragg angle θ_B, i.e., the so-called rocking curve. Fitting of the data set with appropriate functions allows to separate the individual contributions of phase and amplitude gratings to the overall diffraction efficiency and further yields information on a mutual phase shift. With thermally reduced, nominally undoped $\mathrm{LiNbO_3}$ as an example we show our results on the time-resolved determination of the rocking curve in the time regime of 10^{-8} s to 10^2 s with a temporal resolution of up to 10 ns. The gratings are recorded by pulsed laser light ($\lambda = 532$ nm, $\tau = 8$ ns) and are probed in the near-infrared spectral range at $\lambda = 785$ nm. Grating analysis yields the temporal development of phase and amplitude gratings, which originate from optically generated small polarons.

*Financial support by the DFG (Projects IM37/5-1 and GRK 695) is gratefully acknowledged.

DF 13.6 Wed 15:00 Poster A

Photonic Band Structure Analysis of Bi- and Multicontinuous Structures — •Matthias Saba and Gerd Schröder-Turk — Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7B, 91058 Erlangen, Germany

Photonic crystals based on triply-periodic minimal surfaces have recently attracted attention because of their occurence in biological systems, e.g. in butterfly scales or beatle shells. Here we analyse the photonic band structure of bicontinuous surface models (dividing space into two intertwined continuous network domains) and multicontinuous surface models (with three or more continuous network domains), with and without chirality, that are models for self-assembled biological or chemical structures. Triply-periodic surfaces with constant mean curvature H_0 are generated by numerical minimization of a surface energy functional $\int dS(H(r) - H_0)^2$. One or more of these surfaces divide space into interpenetrating networks which are filled with materials of different dielectric constants. The band structures of the resulting bi- and multicontinuous photonic crystals are computed by the frequency domain eigensolver MPB. The aim of this work is to find structures with complete band gaps.

DF 13.7 Wed 15:00 Poster A

Metamaterial hydrogen sensor — •Patrick Mai and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

Hydrogen has gained a substantial amount of interest in recent years and is considered to be a future carrier of energy. However, hydrogen can mix and ignite with air in a wide concentration range - hence monitoring is necessary.

We present an optical hydrogen sensor based on a metamaterial principle. Our stacked sample consists of a gold mirror and palladium nanowires. By tailoring the structural parameters one can tailor the optical properties and achieve a hydrogen-dependent response.

We present temperature- and time-dependent measurement results. Advantages and disadvantages over conventional hydrogen sensors are pointed out, and the development towards an all-optical hydrogen sensor with full seperation of detection electronics and measurement optics will be discussed.

DF 13.8 Wed 15:00 Poster A

Raman scattering of $\mathrm{BiCrO_3}$ thin films: experimental and first-principles studies — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], Silvia Schumann[1], Christian Röder[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

The strong research interest in multiferroic epitaxial films arises from their interesting properties and is stimulated by their potential applications in non-volatile ferroelectric memories or novel multiple state memories and devices based on magnetoelectric effects. Among the Bi-containing perovskite-type transition metal oxides, $\mathrm{BiCrO_3}$ is the least investigated one and the literature is still lacking Raman scattering data. In this work epitaxial thin films of $\mathrm{BiCrO_3}$ were deposited onto $\mathrm{NdGaO_3}$ (110) substrates by pulsed laser deposition. Bulk $\mathrm{BiCrO_3}$ has a monoclinic structure with the space group C2/c below 420 K [1]. The Raman spectra of the $\mathrm{BiCrO_3}$ films were measured from 77 K to room temperature using a UV Labram spectrometer. The 325 nm emission line of a HeCd laser was used for excitation. The assignment of the phonon modes in the Raman spectra of $\mathrm{BiCrO_3}$ was done by comparing the experiments with density functional theory calculations.

[1] A.A. Belik *et al.*, Chem. Mater 20, 3765 (2008).

DF 13.9 Wed 15:00 Poster A

Ab initio study of phonons in $\mathrm{BaTiO_3}$ — •Pavel Ignatiev and Valery Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Ferroelectric $\mathrm{BaTiO_3}$ ceramic is a very important technological material. Its structure, however, can be different from the perovskites ideal cubic phase. Depending on temperature $\mathrm{BaTiO_3}$ can turn to rhombohedral, orthorhombic, tetragonal, cubic and even hexagonal phases. Here we present an ab initio study of various phases of BaTiO3. We report on the optimized lattice parameters, electronic structure and phonons. Ab initio calculations are performed by means of the density functional theory implemented in Quantum Espresso package [1]. Phonons are calculated using the density functional perturbation theory [2]. Polarization-induced LO/TO splitting of phonon branches and Born effective charge tensors are obtained from the first principles using modern polarization theory.

[1] P. Giannozzi et al., J. Phys.: Condens. Matter 21, 395502 (2009).

[2] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. 73, 515 (2001).

DF 13.10 Wed 15:00 Poster A

thermisches Polarisationsrauschen von Silbernatriumnitrit — •Jumna Mehlis — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Germany

Messung des thermischen Polarisationsrauschspektrums in der Umgebung des strukturellen Phasenüberganges eines ferroelektrischen Silbernatriumnitrit-Kristalles

DF 13.11 Wed 15:00 Poster A

The influence of external electric fields on ferroelectric domain lengths in Calcium Barium Niobate — •Urs Heine[1], Klaus Betzler[1], Manfred Burianek[2], and Manfred Muehlberg[2] — [1]Department of Physics, University of Osnabrueck, D-49069 Osnabrueck — [2]Institute of Crystallography, University of Cologne, D-50674 Cologne

We present optical investigations on the novel tungsten bronze type Calcium Barium Niobate (CBN). Using the Czochralski method, [001]-oriented colorless single CBN crystals were grown from the congruently melting composition of 28.1 mole% calcium. The samples with 12 mm in diameter and about 80 mm in length were cut to 2 - 5 mm thickness, and the c-faces were polished to optical quality. Water electrodes were used to connect the c-faces to a high voltage supply, while simultaneously directing an infrared laser beam parallel to the c-axis. When illuminating the crystal, a conical light pattern emerges from the back side of the crystal due to quasi-phase matched second harmonic generation (SHG). The size distribution of the ferroelectric domain structure, contributing to the quasi-phase matching process, manifests itself in the angular intensity distribution of the SHG light pattern. We investigated the field dependent angular intensity distribution, which allows for calculating back on the average domain size, and in particular the mean length of the ferroelectric domains. The influence of ferroelectric aging effects on the domain length was also observed. Monte Carlo simulations were used for fitting generated domain structures with particular mean domain widths and lengths to the measurement data.

DF 13.12 Wed 15:00 Poster A

The local structure of 0.9PZN-0.1PT at high temperature and pressure — •Naemi Waeselmann[1], Boriana Mihailova[1], Bernd Maier[1], Marin Gospodinov[2], and Ulrich Bismayer[1] — [1]Institute of Mineralogy and Petrology, University of HAmburg, Gindelallee 48, D-20146 Hamburg, Germany — [2]Institute of Solid State Physics, Bulgarian Academy of Science, Blvd. Tzarigradsko Chausse 72, 1784 Sofia, Bulgaria

Single crystals of (1-x)Pb(Zn$_{1/3}$Nb$_{2/3}$)O$_3$ (PZN)-xPbTiO$_3$ (PT) show extremely strong direct and converse piezoelectric effect and are considered as one of the most promising materials for next generation electromechanical sensors and transducers. Solid solutions of (1-x)PZN-xPT with a low x-value exhibit rhombohedral symmetry, whereas those with a high x-value have a tetragonal structure, and the morphotropic phase boundary (MPB) is found to be near $x = 0.1$. In situ high-pressure and high-temperature Raman scattering data on 0.9PZN-0.1PT are analysed in order to give a better insight into the atomic arrangements in the vicinity of MPB.

DF 14: Glasses I (Joint Session of DY, DF, CPP)

Time: Wednesday 14:00–17:30 Location: H48

Invited Talk DF 14.1 Wed 14:00 H48

New Approach to the Old Problem: Cooperativity in Dynamics of Glass Forming Systems — •Alexei Sokolov — Oak Ridge National Lab and UT Knoxville, USA

The mechanism behind the steep slowing down of molecular motions upon approaching the glass transition remains a great puzzle. Most of the theories relate this mechanism to the cooperativity in molecular motion. In this talk we present estimates and analysis of the molecular cooperativity in many glass-forming systems. We demonstrate that the cooperativity length scale directly correlates to the dependence of the structural relaxation on volume. This dependence presents only one part of the mechanism of slowing down the structural relaxation. Our analysis reveals that another part, the purely thermal variation of the structural relaxation, does not have a direct correlation with molecular cooperativity. These results call for a conceptually new approach to the analysis of the mechanism of the glass transition and to the role of molecular coopertaivity in slowing down of structural relaxation.

DF 14.2 Wed 14:30 H48

THz Signatures of the Glass Transitions in Polymers — •Marco Reuter[1], Steffen Wietzke[2,3], Christian Jansen[2,3], Tilmann Jung[1], Sangam Chatterjee[1], Wiebke Dempwolf[4], Henning Menzel[4], and Koch Martin[1,3] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Institut für Hochfrequenztechnik, TU Braunschweig, Schleinitzstr. 22, 38106 Braunschweig, Germany — [3]Joint Optical Metrology Center, c/o TU Braunschweig, Fakultät für Elektrotechnik und Informationstechnik, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany — [4]Institut für Technische Chemie, TU Braunschweig, Hans-Sommer-Str. 10, 38106 Braunschweig, Germany

The glass transition temperature of polymers is found with terahertz time-domain spectroscopy. In the region of the glass transition the thermo-quasi-optic coefficient changes noticeably. THz time-domain spectroscopy is a non-destructive and non-contact technique to analyse polymers.

DF 14.3 Wed 14:45 H48

The elusive nature of the Debye process in monohydroxy alcohols: A new approach with ^{2}H-NMR techniques — •Sebastian Schildmann, Catalin Gainaru, and Roland Böhmer — Experimentelle Physik III, Fakultät für Physik, Technische Universität Dortmund

Viscous monohydroxy alcohols, also water, exhibit a so called Debye process in their dielectric spectra. This relaxational feature corresponds to degrees of freedom which are about 100 times slower than those giving rise to the structural rearrangements (α-process). In spite of numerous experimental investigations [1], the nature of these slow "superstructure" relaxation modes is not agreed upon, although it is clear that they are to be related with the presence of hydrogen bonds. The Debye process separates from the structural process if the network is interrupted chemically by diluting or topologically by confining the system in pores. Here butanol diluted with bromobutane was studied with several ^{2}H-NMR techniques. Correlation times measured with stimulated-echo experiments are compared with data obtained from dielectric spectroscopy [2]. Spin-lattice relaxation times were measured for O-D deuterated samples to check how the hydrogen bonds affect the dynamics.

[1] M. Poeschl & H.G. Hertz, J. Phys. Chem. 98, 8195 (1994).

[2] T. El Goresy & R. Böhmer, J. Chem. Phys. 128, 154520 (2008).

DF 14.4 Wed 15:00 H48

Relaxation Kinetics of Nanoscale Indents in a Polymer Glass — •Armin Knoll, Dorothea Wiesmann, Bernd Gotsmann, and Urs Duerig — IBM Research - Zurich, 8803 Rueschlikon, Switzerland

Nanometer scale indents have been written in a cross-linked polystyrene sample, and their relaxation has been studied at annealing temperatures well below the glass transition of the polymer. The indents represent a highly nonequilibrium state of the polymer which is subjected to mechanical stress of up to 0.4 GPa and thermal quench rates on the order of 10^8 K/s during writing. It is shown that the relaxation towards equilibrium evolves logarithmically over more than 10 orders of magnitude in time. The relaxation kinetics are accurately described in terms of a thermally activated process with an energy barrier whose magnitude decreases linearly with the distance from equilibrium [1].

[1] A. Knoll, D. Wiesmann, B. Gotsmann, and U. Duerig, *Phys. Rev. Lett.*, **102**, 117801 (2009)

DF 14.5 Wed 15:15 H48

Studying the dynamics of water molecules on a complex lattice: KOH doped tetrahydrofuran clathrate hydrate — •Helge Nelson[1], Catalin Gainaru[1], Andre Nowaczyk[1], Sebastian Schildmann[1], Burkhard Geil[2], and Roland Böhmer[1] — [1]Experimentelle Physik III, Fakultät für Physik, TU Dortmund — [2]Institut für Physikalische Chemie, Universität Göttingen

Because of kinetic hindrance during the freeze-out of the protons in clathrate hydrates an orientational glass transition is observed. By adding minute amounts of ionic dopants, e.g., KOH, the timescale of ordering can be accelerated significantly and an ordered phase is reached [1]. We applied a combination of dielectric and ^{2}H-NMR techniques to study the lattice dynamics of the water molecules in a temperature range from 30 K to 260 K. The ^{2}H-NMR techniques include temperature dependent lineshape analysis, measurement of relaxation times, and the stimulated-echo technique. This combination allows the observation of dynamics in a broad frequency and temperature window. We found several reorientational processes on the lattice, which are absent in the undoped sample. In addition we were able to detect the phase transition into the proton ordered phase with both dielectric and NMR measurements close to 62 K.

[1] see O. Yamamuro, et al., Physica B 213, 405 (1995) and references cited therein.

15 min. break

Invited Talk DF 14.6 Wed 15:45 H48

Slow domains percolation in polymer melts and blends close to the glass transition: a unifying concept regarding bulk dynamics, dynamics in the vicinity of interfaces, and the physical properties of nanocomposites — •Didier R. Long — Laboratoire Polymères et Matériaux Avancés; CNRS/Rhodia; F-69192 Saint Fons, France.

Experiments have demonstrated over past 15 years that the dynamics in liquids close to and below the glass transition temperature is strongly heterogeneous, on the scale of a few nanometers and, independantly, that the glass transition temperature in the vicinity of interfaces can be very different from that in the bulk, with shifts either positive or negative depending on the interaction between the polymer and the interface. By considering thermally induced density fluctuations in the bulk, we proposed that the 3-D glass transition is controlled by the percolation of small domains of slow dynamics, which allows to explain the heterogeneous dynamics close to Tg. This model allowed then for interpreting a priori unrelated features of polymer dynamics: 1) the main feature of confinement effects on the dynamics; 2) Unique reinforcement, plastic and recovery behaviour of nano-filled elastomers; 3) ageing and rejuvenating dynamics polymeric liquids; 4)case II diffusion, which is how a solvent penetrates and finally melts a glassy polymer matrix.

Regarding these various issues, I will put the emphasis on how percolation of slow domains is key for explaining their main features.

DF 14.7 Wed 16:15 H48

Glass Transition of Molecules Sorbed in Zeolites — Özlen F. Erdem[1], •Dieter Michel[2], Pavel Sedykh[2], and Jürgen Haase[2] — [1]Max-Planck-Institute of Bioinorganic Chemistry, Stiftstraße 34-36, 45470 Mülheim an der Ruhr, Germany — [2]University of Leipzig, Faculty of Physics and Earth Sciences, Linnéstraße 5, 04103 Leipzig, Germany

Proton MAS NMR, nuclear spin relaxation, and deuteron NMR spectroscopy are combined to study the mobility of ethylene glycol molecules sorbed in various zeolites over a wide temperature range. The results obtained will be also compared with broad-band dielectric measurements and with previous extensive dielectric studies by Kremer *et al.* [1]. The main question is whether the adsorbed species show a so called single-molecule behavior characterized by an Arrhenius type temperature dependence of the correlation times or the respective dielectric relaxation times. In contrast, a Vogel-Fulcher-Tammann (VFT) type temperature dependence of the dielectric relaxation rate would point out collective motions and is typical for the appearance of a glass-transition. An important question is the competition between molecule-to-molecule and molecule-to-surface interactions.

[1] F. Kremer, A. Huwe, M. Arndt, P. Behrens, W. Schwieger, J. Phys. Cond. Mat. **11**, A175-A188 (1999); A. Huwe, F. Kremer, J. Kärger, P. Behrens, W. Schwieger, G. Ihlein, O. Weiss, F. Schuth, J. Mol. Liquids **86**, 173-182 (2000).

DF 14.8 Wed 16:30 H48

Molecular glass formers in hard and soft confinement probed by ^{31}P and ^{2}H NMR — •Daniel Bock, Sabine Gradmann, and Ernst Rössler — Experimentalphysik II, Universität Bayreuth

Low molecular glass formers confined in nanoporous silica matrices (hard confinement) are investigated by different ^{31}P and ^{2}H NMR methods such as spin-lattice-, spin-spin relaxation, line-shape and stimulated echo decay.

Decreasing the radius of the pores pronounced dynamic heterogeneities are observed. For example, the correlation function revealed by the stimulated echo exhibits a quasi-logarithmic decay in contrast to Kohlrausch decay in the bulk. As shown by 2D spectra the dynamic heterogeneities are transient in time, i.e., we observe exchange between slow and fast molecules. The effects are explained by assuming dynamics being inhomogeneous in space; that is the dynamics given by a correlation time $\tau(r)$ depend on the distance r from the confining wall.

Similar NMR features are found for low molecular additives dissolved in polymer matrices (soft confinement). The additive dynamics are decoupled from those of the polymer, and liquid-like additive dynamics are revealed below T_g, i.e., in a solid polymer matrix. Again, strongly stretched correlation functions are observed.

DF 14.9 Wed 16:45 H48

Quantitative Lineshape Analysis for 1D- and 2D-Spectra of Amorphous Materials — •Jörn Schmedt auf der Günne, Sabarinathan Venkatachalam, Johannes Weber, and Yamini Avadhut — Department of Chemistry, Munich University (LMU), Germany

NMR is quantitative, is an often stated feature in magnetic resonance. In ^{1}H solid-state NMR the results from simple MAS experiments can be disappointing though. We present a model study [1] which identifies and quantifies different sources of errors and a new strategy which gives reliable results even under low resolution conditions.

A second aspect will be 2D deconvolution of the lineshapes of amorphous/glassy materials. We analyze the unexpected splittings in the 2D lineshape of many typical glasses with a new analytical fitting function. Based on these findings we suggest a structural model based on different subunits, which should also find their imprint in bulk properties.

[1] Y.S.Avadhut, D.Schneider, J.Schmedt auf der Günne, J. Magn. Reson. 201 (2009) 1-6.

DF 14.10 Wed 17:00 H48

Low-Frequency Excess Contribution in Simple Liquids Revealed by Fast Field Cycling NMR — •Roman Meier, Axel Herrmann, Robert Kahlau, Danuta Kruk, and Ernst Rössler — Experimentalphysik II, Universität Bayreuth, Germany

The main relaxation (α-relaxation) of simple liquids studied by dielectric spectroscopy is well described by a Cole-Davidson (CD) susceptibility. In particular the low-frequency limit follows a Debye behavior $\chi''_{DS} \propto \omega^1$. Applying fast field cycling (FFC) ^{1}H NMR and transforming the spin-lattice dispersion data T_1 into the susceptibility representation $\chi''_{NMR} \propto \nu/T_1$ we have discovered a low-frequency excess contribution for systems like glycerol and its homologues as well as fluoroaniline. The CD function fails to describe the data due to a retarded transition to the limit ω^1, i.e., a "shoulder" is observed on the low frequency side of the a-relaxation peak ($\omega\tau_\alpha < 1$) possibly reflecting a slower relaxation process. Actually only a few liquids like o-terphenyl and tristyrene studied by FFC NMR do not show this phenomenon. Collecting dispersion data over a large temperature range, the relaxation strength of the excess contribution is specified quantitatively. Measurements of dilution series of propylene glycol in deuterated chloroform proved an intermolecular origin of the excess contribution. Dilution experiments of deuterated in protonated glycerol suggest this additional contribution being also fully reflected by sole intramolecular spin-spin vectors. A possible explanation of this effect are transient molecular clusters due to chemical interactions (e.g. H-bonds).

DF 14.11 Wed 17:15 H48

Glass transition of colloidal particles with long-ranged interactions in two dimensions — •David Hajnal, Martin Oettel, and Rolf Schilling — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

We study the glass transition behavior of binary mixtures of colloidal particles with long-ranged dipolar interactions in two dimensions in the framework of mode-coupling theory (MCT). We first present a minimal model for the theoretical description of the thermodynamic properties of the experimental system studied by König et al. [1]. By applying MCT to this model, we determine its glass transition diagram, i.e. we calculate the variation of the critical interaction strength upon composition changes. Finally, we compare the mixing effects predicted by MCT for this model to both experiments [1] and MCT results for binary mixtures of hard disks [2].

[1] H. König, R. Hund, K. Zahn, and G. Maret, Eur. Phys. J. E **18**, 287 (2005).

[2] D. Hajnal, J. M. Brader, and R. Schilling, Phys. Rev. E **80**, 021503 (2009).

DF 15: Optical and nonlinear optical properties, photonics II

Time: Thursday 10:00–12:50 Location: H11

Invited Talk DF 15.1 Thu 10:00 H11

Photons meet sound waves — •Jan K Krüger and Roland Sanctuary — University of Luxembourg, Laboratoire de physique des matériaux, Luxembourg, Luxembourg

High performance Brillouin spectroscopy is an optical method which is predominantly used for studies of the mechanical behaviour of condensed matter at hypersonic frequencies. Brillouin spectroscopy works contact- and destruction-less but needs rather transparent samples. The latter prerequisite is for soft matter no real restriction, especially, because the samples can be made thin. The typical probe volume is 10-8 cm3. After a short introduction to the theoretical background a description of the experimental technique will be given including an introduction to modern acoustic microscopy. The wide spectrum of useful applications of Brillouin spectroscopy will be demonstrated using examples from synthetic and biological polymers.

5 min. break

DF 15.2 Thu 10:45 H11

Optical properties of Calcium Barium Niobate — •Urs Heine[1], Klaus Betzler[1], Manfred Burianek[2], and Manfred Muehlberg[2] — [1]Department of Physics, University of Osnabrueck, D-49069 Osnabrueck — [2]Institute of Crystallography, University of Cologne, D-50674 Cologne

We report on optical measurements on the novel tungsten bronze type Calcium Barium Niobate. [001]-oriented transparent and colorless single crystals were grown by the Czochralski method with dimensions of 12 mm in diameter and about 80 mm in length. With its relatively high Curie temperature of about 538 K for the congruently melting composition of 28.1 mole% calcium and its high nonlinear coefficients, CBN is a promising material for future applications. Recent experiments revealed, that the application of an external electric field of several kV/cm to CBN at room temperature leads to an increasing opacity of the sample. This might be a drawback considering the future usability of CBN in optical systems. We present investigations on the transmittance behaviour of CBN under external electric fields, demonstrating the erasement of the clouding without affecting the polarization. Experiments have been performed at temperatures ranging from room temperature to approximately 480 K. When heating up the sample, its colorless appearance changes to a light yellow, which can be attributed to a shift of the band edge to longer wavelengths with increasing temperature. To further investigate the transmittance properties of CBN, measurements of the band edge under various temperatures up to the ferroelectric phase transition have been performed.

DF 15.3 Thu 11:05 H11

Investigation of nonlinear optical effects in strontium barium niobate — •Alexander Niemer, Rainer Pankrath, and Klaus Betzler — University of Osnabrück, Department of Physics, Barbarastr. 7, 49076 Osnabrück

The ferroelectric relaxor and optical nonlinear material strontium barium niobate (SBN) shows some very interesting effects in the nonlinear generation of light and offers the possibility to study the interaction between the luminescence of rare earth ions and the nonlinear processes.

The possibility of getting radially polarized light from an SBN crystal is investigated. By excitation with an optical parametrical oscillator radially polarized white light can be generated. In the literature [1] it is shown, that such light can be focused to a smaller spot size than linear or azimutal polarized light. At the moment an about 10% smaller spot size is realized.

Further the luminescence from different rare earth impurities is studied. To understand the processes which are responsible for the upconversion the dependency of time and excitation energy was investigated. For erbium and ytterbium an anomalous dependency of the fluorescence decay time on the dopant concentration is found. Because ytterbium doped SBN shows a very high luminescence intensity the luminescence light could be used for other nonlinear processes like, e.g. sum frequency generation.

[1] R. Dorn, S. Quabis, G. Leuchs: Optics Communications 179, 1-7 (2000)

DF 15.4 Thu 11:25 H11

Temperaturabhängigkeit des Optischen Schadens in Lithiumniobat-Kristallen* — •Niklas Waasem[1], Fabian Lüdtke[1], Mercedes Carrascosa[2] und Karsten Buse[1] — [1]Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn, Deutschland — [2]Departamento de Física de Materiales C-IV, Universidad Autónoma de Madrid, Campus Cantoblanco, E-28049, Madrid, España

Lithiumniobat-Kristalle besitzen große nichtlineare optische Koeffizienten, die Frequenzkonversion von Laserlicht ermöglichen. Oft behindert der photorefraktive Effekt den Einsatz der Kristalle jedoch erheblich: Unkontrollierte lichtinduzierte Brechungsindexänderungen zerstören die Phasenanpassung und führen zu einer Verzerrung des Strahlprofils. Dieses unerwünschte Auftreten des photorefraktiven Effekts wird „Optischer Schaden“ genannt. Seit seiner Entdeckung vor 50 Jahren ist der Effekt nicht vollständig unter Kontrolle gebracht worden.

Das Ziel unserer Untersuchungen ist ein tieferes Verständnis des Optischen Schadens zu erlangen. Hierzu wird die Schwellintensität für das Einsetzen des Optischen Schadens in Abhängigkeit von der Kristalltemperatur anhand der Verzerrung eines durch den Kristall transmittierten Laserstrahls gemessen. Wir finden ein Arrhenius-Verhalten mit der Aktivierungsenergie 0.5 eV. Ein kürzlich entwickeltes Modell zur Erklärung des Optischen Schadens von Carrascosa et al., welches auf zwei photorefraktiven Zentren basiert, kann die Ergebnisse gut erklären. *Unterstützt von der Deutschen Forschungsgemeinschaft, der Deutschen Telekom AG und dem DAAD.

5 min. break

DF 15.5 Thu 11:50 H11

Ionendurchstrahltes Lithiumniobat: Änderung optischer und elektrischer Materialeigenschaften* — •Niels Lennart Raeth, Lena Jentjens, Konrad Peithmann und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn

Lithiumniobat findet vielfache Anwendungen in Wissenschaft und Technik, insbesondere in optischen Bereichen. Um die Vorzüge des Materials vollständig ausnutzen zu können, ist eine genaue Kenntnis und die Möglichkeit zur Modifikation der Materialparameter erstrebenswert.

Wird Lithiumniobat mit schnellen ^{3}He-Ionen bei einer Energie von 41 MeV durchstrahlt, können entscheidende Materialeigenschaften gezielt großvolumig und strukturiert geändert werden. In der durchstrahlten Region werden langzeitstabile Brechungsindexänderungen, sowie eine Herabsetzung der Koerzitivfeldstärke beobachtet. Darüber hinaus zeichnet sich nach der Bestrahlung eine erhöhte Leitfähigkeit des Materials sowie eine erhöhte Dichte an Nukleationskeimen ab.

*Gefördert durch die Deutsche Forschungsgesellschaft (FOR557,R2)

DF 15.6 Thu 12:10 H11

Transient light–induced absorption in thermally reduced, periodically poled lithium niobate doped with yttrium — •Bettina Schoke[1], Mirco Imlau[1], Christoph Merschjann[2], Garbor Corradi[3], Katalin Polgar[3], and Inna Naumova[4] — [1]Physics Department, University of Osnabrück, Germany — [2]Helmholtz-Zentrum Berlin GmbH, Germany — [3]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences Budapest, Hungary — [4]Physics Department, Moscow State University, Russia

Excitation and recombination processes of small polarons are studied in thermally reduced, periodically poled $LiNbO_3$ doped with Y (PPLN:Y). The reduction treatment creates bipolarons (Nb_{Li}^{4+}:Nb_{Nb}^{4+}) which are stable at room temperature. They may be dissociated optically into small bound (Nb_{Li}^{4+}) and free (Nb_{Nb}^{4+}) polarons (”optical gating”). The light-induced absorption arising from the population and depopulation of these centers is measured time–resolved via transient absorption spectroscopy in the blue and red spectral range after optical excitation with intense laser pulses ($\lambda = 532\,\mathrm{nm}$, $t = 8\,\mathrm{ns}$). Besides dissociation and relaxation of bipolarons the investigations also indicate the presence of photo-induced hole polarons (O^-) with comparatively longer lifetime. The findings can be explained by a periodic spatial modulation of the Nb_{Li}^{5+} antisite concentration and of the degree of reduction. Both modulations most likely result from a periodic incorporation of Y ions on Li sites. *Financial support by the DFG (IM 37/5-1, GRK695) is gratefully acknowledged.

DF 15.7 Thu 12:30 H11

Tunability of photoswitchable ruthenium sulfoxide compounds on the basis of ligand substitution — •Sebastian Eicke, Volker Dieckmann, Kristin Springfeld, and Mirco Imlau — Deparment of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Photoswitchable ruthenium sulfoxide compounds provide a light-induced linkage isomerization in combination with pronounced changes in characteristic optical properties.

As representative of the ruthenium sulfoxide group the molecular compound $[\mathrm{Ru(bpy)_2(R\text{-}OSO)}]^+$ (OSO: 2-methylsulfinylbenzoate) can be tuned in its optical properties by the substitution of the photoswitchable ligands (R=Bn, BnCl, BnMe). These modified sulfoxides were studied in respect to their photochromic properties and kinetics of the generation and relaxation of the light-induced isomers. The kinetics were determined by pump-probe technique and show in each case two reversible termal decay processes following Arrhenius law. The two photo-excited states offer lifetimes in the magnitude of $\tau_1 \approx 10^3$ s and $\tau_2 \approx 10^4$ s at room temperature with activation energies about $E_{\mathrm{A,I}} = 0.72$ eV to 0.92 eV and $E_{\mathrm{A,II}} = 0.8$ eV to 1.00 eV. Another representative of the photoswitchable sulfoxides is the $[\mathrm{Ru(bpy)_2(pySO)}]^{2+}$ compound. This molecule is the first sulfoxide which allows for reversible switching between the ground and metastable states by light exposure. With this compound the sulfoxides are highly qualified for optical data storage on a molcular scale. Financial support by the DFG (GRK 695).

DF 16: Phase Transitions

Time: Thursday 14:00–15:25 Location: H11

Invited Talk DF 16.1 Thu 14:00 H11

Succesive phase transitions in $(\mathrm{Gua})_4\mathrm{SO_4Cl_2}$ crystal - dielectric, pyroelectric, dilatometric and optical studies — •Zbigniew Czapla[1,2], Artur Rokosa[1], Slawomir Dacko[1], and Boguslaw Kosturek[1] — [1]Institute of Experimental Physics, University of Wrocław, pl M. Borna 9, 50-204 Wrocław, Poland — [2]Department of Physics, Opole Unoversity of Technology, Ozimska 75, 45-271 Opole, Poland

Te studies of dielectric and pyroelectric properties along the ferroelectric a - axis, optical observation along the b-axis and dilatometric measurements along the a-, b- and c- axes for of $(\mathrm{Gua})_4\mathrm{SO_4Cl_2}$ crystal were performed in the temperature range 330-380 K covering the phase transitions region at various heating/cooling rates regime. Presented studies on heating run at the rate 0.01 K/min showed the successive phase transitions at $T_2 = 353$ K and $T_1 = 357.5$ K with the symmetry changes according to the scheme: orthorhombic(III) - orthorhombic(II) - tetragonal (I) and on cooling: tetragonal (I) - orthorhombic (II). The dielectric, pyroelectric, dilatometric and optical studies allowed to conclude that the phase transition III-II at T_2 is characterized by slow kinetics. The studies of permittivity and dimensions changes of the samples which were kept at constant temperature inside of phase II during 180 min gave some detailed information about kinetics of III-II phase transition. The time changes of permittivity and dimensions were describe using Avrami model.

5 min. break

DF 16.2 Thu 14:45 H11

Common characteristics of displacive and relaxor ferroelectrics — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

The long standing classification scheme of ferroelectrics into either relaxor or displacive ones (the phase transition is driven by a soft phonon mode) is shown to be too restrictive since a smooth crossover between them exists which even admits for a coexistence of both phenomena. This crossover and coexistence is a consequence of the varying density of polar nanoregions due to different doping levels of the respective system. The formation of polar nanoregions is attributed here to intrinsic local modes (ILM) in terms of discrete breathers. Consequences for the dynamics, temperature effects and line width broadening are discussed.

DF 16.3 Thu 15:05 H11

High-pressure structure of Pb-based relaxor ferroelectrics — •Bernd J. Maier[1], Ross J. Angel[2], William G. Marshall[3], Boriana Mihailova[1], Carsten Paulmann[1], Jens M. Engel[4], Marin Gospodinov[5], Anna-Maria Welsch[1], Dimitrina Petrova[5,6], and Ulrich Bismayer[1] — [1]Mineralogisch-Petrographisches Institut, Universität Hamburg — [2]Crystallography Laboratory, Virgina Tech, Blacksburg, USA — [3]ISIS neutron facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, UK — [4]Institut für Werkstoffwissenschaft, Technische Universität Dresden — [5]Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria — [6]South-West University “Neofit Rilski”, Blagoevgrad, Bulgaria

The pressure-induced phase transitions that occur in the perovskite-type relaxor ferroelectric $\mathrm{PbSc_{0.5}Ta_{0.5}O_3}$ (PST) and $\mathrm{Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3}$ (PST-Ba) were studied with combined neutron powder diffraction and single-crystal X-ray diffraction. An increase in the intensities of $h,k,l =$ all odd reflections is observed while the intensity of h,h,h peaks, $h = 2n+1$, does not change with pressure, indicating a glide-plane pseudo-symmetry of the structural distortion along the $\langle 111 \rangle$ cubic directions. Rietveld refinement to the neutron powder data shows that the high-pressure phase has either $R\bar{3}c$ or $R\bar{3}$ symmetry, depending on whether the presence of 1:1 octahedral cation ordering is neglected or taken into account, and comprises anti-phase octahedral tilts of type $a^-a^-a^-$ that continuously evolve with pressure.

DF 17: Nano- and microstructured dielectrics

Time: Thursday 15:30–17:30 Location: H11

DF 17.1 Thu 15:30 H11

Low-Voltage Nano-Domain Writing in He-Implanted Lithium Niobate Crystals — •Martin Lilienblum[1], Avishai Ofan[2], Ákos Hoffmann[1], Ophir Gaathon[2], Lakshmanan Vanamurthy[3], Sasha Bakhru[3], Hassaram Bakhru[3], Richard Osgood Jr.[2], and Elisabeth Soergel[1] — [1]Institute of Physics, University of Bonn, 53115 Bonn, Germany — [2]Center for Integrated Science and Technology, Columbia University, New York NY 10027, USA — [3]College of Nanoscale Science and Engineering, State University of New York at Albany, Albany NY 12222, USA

A scanning force microscope tip is used to write ferroelectric domains in He-implanted single-crystal lithium niobate and subsequently probe them by piezoresponse force microscopy. Investigation of cross-sections of the samples showed that the buried implanted layer, $\sim 1\,\mu$m below the surface, is non-ferroelectric and can thus act as a barrier to domain growth. This barrier enabled stable surface domains of $< 1\,\mu$m size to be written in $500\,\mu$m-thick crystal substrates with voltage pulses of only 10V applied to the tip.

DF 17.2 Thu 15:50 H11

Surface-charge effects of nanocrystalline lithium niobate* — •Daniel Schütze, Bastian Knabe, and Karsten Buse — Universität Bonn, Wegelerstr. 8, 53115 Bonn

As a ferroelectric material, lithium niobate exhibits a spontaneous polarization, which leads to charged c-faces. In the most simple picture, these charges can be fully compensated by various compensation mechanisms. Yet, investigations of surface charges show that this compensation is incomplete. Remaining surface charges lead to a finite dipole moment of lithium niobate nanoparticles. We analyze this dipole moment and its dependence on dopants and dopant concentration by measuring the orientation of nanoparticles in liquids upon application of electric fields.

* Financial support by the Deutsche Forschungsgemeinschaft and the Deutsche Telekom AG is gratefully acknowledged.

DF 17.3 Thu 16:10 H11

The novel polarization patterns in BaTiO$_3$ nanowires from first principles — •Jiawang Hong[1,2], Gustau Catalan[1,3], Daining Fang[2,4], Emilio Artacho[1,5], and James F. Scott[1,6] — [1]Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, UK — [2]AML,Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, P. R. China — [3]ICREA and Centre d'Investigacio en Nanociencia i Nanotecnologia (CIN2), Campus UAB, Bellaterra, Spain — [4]LTCS, College of Engineering, Peking University, Beijing 100084, P.R.China — [5]Donostia International Physics Centre, Universidad del Pais Vasco, 20080 San Sebastian, Spain — [6]Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK

Based on first principles calculations, the behaviour of the cross-sectional polarization field is explored for thin BaTiO$_3$ nanowires with different surface terminations. The unusual and interesting polarization patterns are discovered in these wires, beyond the known patterns in ferroelectric nanostructures. It is found that these new patterns result from the competition of surface effects and edge effects. The critical size of nanowires with different surface terminations is also investigated.

DF 17.4 Thu 16:30 H11

Size Effects in Fine Barium Titanate Particles — •Pavel Sedykh[1], Dieter Michel[1], Elena V. Charnaya[2], and Jürgen Haase[1] — [1]University of Leipzig, Faculty of Physics and Earth Sciences, Linnéstraße 5, 04103 Leipzig, Germany — [2]St.Petersburg State University, Faculty of Physics, Ul'yanovskaya street 1, 198504 St.Petersburg, Russia

^{137}Ba NMR spectroscopy is very suitable to study size effects in very fine particles of barium titanate where particle sizes varied between 155 and 15 nm. The NMR measurements were carried out within the temperature range of the ferroelectric tetragonal phase and allowed us to deduce information about the spontaneous electric polarization. The fine particles are composed of an "ordered" part showing a tetragonal structure and a so called "disordered" part. The "ordered" part reveals a first order phase transition and a temperature dependence of the spontaneous polarization which may be described by a power law similar as predicted by the Landau theory but the phase transition temperature becomes slightly lower with decreasing particle diameter and the exponent changes from 1/2 to about 1/3. The applicability of the core-shell model is discussed and the thickness of the shell is estimated. The shell thickness was shown to strongly decrease with decreasing particle size below 50 nm. Therefore, the applicability of other structural models is also discussed.

DF 17.5 Thu 16:50 H11

Conductivity of $BaTiO_3$ metallic composites below the percolation threshold due to finite size effects — •Hans Lustfeld[1] and Martin Reissel[2] — [1]IFF-1, Forschungszentrum Jülich, D52425 Jülich — [2]Fachhochschule Aachen, Abteilung Jülich, D52428 Jülich

The high dielectric permittivity ϵ of $BaTiO_3$ can be enhanced further by adding metallic nanoparticles, e.g. Ni[1, 2] or Ag[3](,size of particles $\approx 10 \cdot 10^{-9}m$). This enhancement becomes arbitrarily high at the concentration c_p of the percolation threshold[4]. Therefore it can be the aim to get very close to c_p. $BaTiO_3$ is an insulator, and if finite size effects can be neglected, the d.c. conductivity remains zero below c_p. However, modern **M**ulti **L**ayer **C**eramic **C**apacitors (MLCC's) have a layer thickness of about $1 - 5 \cdot 10^{-6}m$ only[5], finite size effects become important and lead to increasing finite conductivities when approaching c_p from below. Here we present calculations for the conductivity in the brick layer model[6] and for a modification of the brick-layer model. A main result obtained for both these models is an exponentially strong increase of the d.c. conductivity, as soon as the concentration increases beyond c_{crit}. The concentration c_{crit} depends sensitively on the size of the nanoparticles and is about 10% smaller than c_p for typical sizes.

[1] C. Pithan et.al., Int. J. Mater. Res. **97**, 5 (2006)
[2]Y-C. Huang et.al., J. Am. Ceram. Soc., **90**, 1438 (2007)
[3]Y.Cheng et.al., Appl. Phys. Lett. **91**, 252903 (2007)
[4]W.T. Doyle, J. Appl. Phys. **85**, 2323 (1999)
[5]S. Halder et.al., J. Sol-Gel. Sci. Techn. **42**, 203 (2007)
[6]N.J. Kidner et.al., J. Am. Ceram. Soc. **91**, 1733 (2008)

DF 17.6 Thu 17:10 H11

Dielectric analysis of dispersed particles in composites of unknown microstructure — •Béatrice Hallouet, Carsten Volz, and Rolf Pelster — Universität des Saarlandes, FR 7.2 Experimentalphysik, D–66123 Saarbrücken, Germany

In general, the details of the microstructure in nanocomposites is unknown. Nevertheless there is a need to determine the intrinsic properties of the dispersed phase from the measured effective properties of the system. We present a method to extract at least a partial information using basic physical considerations, among other things energy conservation. The procedure is tested for composites consisting of a solid polymer filled with semi-conductive particles (Ga As in a epoxy resin) using broadband dielectric spectroscopy. From the measured dielectric spectra, which show polarisation peaks (MWS polarisation), we obtain boundaries for the permittivity and the conductivity of the particles.

DF 18: Glasses II (Joint Session of DY, DF, CPP)

Time: Thursday 9:45–12:30 Location: H38

DF 18.1 Thu 9:45 H38

Dynamics of soft spheres beyond the hard-sphere limit — •Michael Schmiedeberg and Andrea J. Liu — University of Pennsylvania, Department of Physics and Astronomy, 209 South 33rd Street, Philadelphia, PA 19104-6396, USA

In the limit of low pressures the dynamics of model glass-forming liquids with finite-ranged repulsive interactions are universal. In that limit, where the product of the pressure and the particle volume is small compared to the interaction energy, soft sphere systems behave as hard spheres, so that the dynamics correspond to those of the hard-sphere glass transition and depend only on the ratio of temperature to the product of pressure and the particle volume. However, at higher pressures relative to the interaction energy, there are deviations from this universal behavior that depend on the inter-particle potential. We consider a bidisperse system consisting of soft spheres that repel each other according to a power law potential δ^α where δ is the particle overlap. By using molecular-dynamics simulations, we determine relaxation times as a function of temperature and pressure. We find that the deviations from hard-sphere behavior can be collapsed onto a single curve that depends on $p^{1/\alpha}$.

DF 18.2 Thu 10:00 H38

Correlation between the Diffusion Dynamics and Vibrational Modes of a Model Glass Former — •Oliver Rubner and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstr. 30, D-48149 Münster, Germany.

In this work we investigate the vibrational modes from computer simulations on a 65 particle binary Lennard-Jones Mixture (BMLJ65) and compare them with the self diffusion dynamics of the particles. As a measure for the dynamics we use the propensities per particle as obtained from an isoconfigurational ensemble which has been introduced by Harrowell (PRL 93, 135701 (2004))

The diffusion dynamics can also be explained in terms of waiting times of the system in inherent structures or metabasins. We compare these waiting times to the vibrational frequencies of the corresponding inherent structures. From this analysis we present the time dependence of the vibrational frequencies which can give some insight into the underlying potential energy surface on which the motion of the system takes place.

DF 18.3 Thu 10:15 H38

Assessing the predictive power of the Reverse Monte Carlo Method for amorphous systems — •Christian Robert Müller[1], Michael Schuch[2], and Philipp Maass[2] — [1]Theoretical Physics II, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [2]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany.

The quality of structural models generated by the Reverse Monte Carlo (RMC) method in a typical application to amorphous systems is investigated. To this end diffraction data from a molecular dynamics (MD) simulation of a lithium silicate glass are calculated and used to generate RMC models with different protocols and starting configurations. This allows us to directly compare structural properties of the RMC models with the original MD structures and hence assess the predictive power of the RMC method. It is found that partial distribution functions and properties on small length scales are well reproduced by the RMC modeling. However, properties in the medium-range order, as, for example, ring size distributions are not well captured. We further show that certain medium-range order features of the RMC models can be a mere consequence of the chosen starting configuration when using commonly applied RMC protocols. Due care therefore has to be exercised when extracting structural features from RMC models in the medium-range order regime and when using corresponding information as a basis for subsequent studies of ion transport properties.

DF 18.4 Thu 10:30 H38

Dielectric noise pattern of the Debye- and α-process in a monohydroxy alcohol — •Tobias Gamp, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Based on the validity of the fluctuation dissipation theorem, dielectric polarization noise spectroscopy allows to measure the dielectric function of a sample electrically non-driven. 2-Ethyl-1-hexanol is one of the prototypical and widely studied glass-forming liquids showing a Debye-like relaxation and the α-peak, the latter associated with the structural relaxation. Since the Debye process is practically invisible in caloric measurements but prominent in conventional dielectric spectroscopy the question whether it could be caused by the presence of electric fields is debated. We show dielectric noise spectra - both voltage and current power spectral densities - and conventional dielectric spectra. Within our experimental resolution and the validity of the fluctuation dissipation theorem both sets of data are in agreement, indicating that the presence of an external field is not necessary for the occurrence of such a Debye peak.

DF 18.5 Thu 10:45 H38

Glass transition in high dimensions — •Bernhard Schmid and Rolf Schilling — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

We have studied the glass transition of hard spheres with diameter σ for dimensions $d \to \infty$ in the framework of mode-coupling theory (MCT). Assuming that the direct correlation function equals the Mayer function in the limit of high dimensions, we have solved numerically the MCT equations [1] up to $d = 800$. The numerical results for the critical collective and self nonergodicity parameters $f_c\,(k;d)$ and $f_c^{(s)}\,(k;d)$ exhibit no Gaussian k-dependence even for $d = 800$. Instead they can be represented by a master function, which vanishes for $k\sigma > \hat{k}_0 d^{3/2}$ with $\hat{k}_0 \cong 0.15$. Inspired by these results, we were able to prove analytically that $f_c\,(k;d)$ converges to $f_c^{(s)}\,(k;d)$ for $k\sigma = O\,(d)$ and $d \to \infty$ and that the critical packing fraction is given by $\varphi_c\,(d) \sim d^2 2^{-d}$. The non-Gaussian character of $f_c\,(k;d)$ and $f_c^{(s)}\,(k;d)$ implies that the hard sphere glass at $\varphi_c\,(d)$ is not a harmonic solid, even in the limit of high dimensions.

[1] M. Bayer, J.M. Brader, F. Ebert, M. Fuchs, E. Lange, G. Maret, R. Schilling, M. Sperl and J.P. Wittmer, Phys. Rev. E **76**, 011508 (2007)

DF 18.6 Thu 11:00 H38

Brownian dynamics simulation of extensional shear flow in dense colloidal hard-sphere systems — •Olaf Herbst[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Using a novel algorithm based on on event-driven MD simulations adapted for Brownian dynamics, we examine an extensional flow of colloidal particles with periodic boundary conditions. We study the slow dynamics of dense hard-sphere systems when shear rates are high enough to interfere with the slow (alpha) relaxation time. Characteristic features such as the mean-square displacement as a function of time will be discussed for a variety of system parameters.

DF 18.7 Thu 11:15 H38

The influence of the method of glass preparation and ambient conditions on diffusion of alkaline-earth ions in mixed cation glasses — •Michael Grofmeier and Hartmut Bracht — Institut für Materialphysik, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster

Diffusion of alkaline-earth ions in mixed alkali (A) alkaline-earth (M) glasses of the composition xA2O*(3-x)MO*4SiO2 with 0<x<3 was investigated by means of the radiotracer diffusion technique below the respective glass transition temperatures. Our previous studies reveal a distinct dependence of the diffusion behavior of the alkaline-earth ions on the composition x and type of cations in the glass. Additional experiments on the alkaline-earth ions mobility in sol-gel derived glasses of the same composition were performed in this work in order to determine whether the mixed cation effect in alkali-alkaline-earth silicate glasses also holds for sol-gel derived thin glass films. We found that the diffusion behavior of cations in mixed cation silicate glasses is independent of the way of glass preparation. Further diffusion measurements under reducing atmosphere demonstrate a retarded mobility of the alkaline-earth cations.

DF 18.8 Thu 11:30 H38

Crystallization and structural investigation of Eu-doped fluorozirconate-based glass ceramics. — •Christian Passlick[1], Bernd Ahrens[1,2], Bastian Henke[1,2], Jacqueline A. Johnson[3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA

A series of Eu-doped fluorozirconate-based glass ceramics has been developed for medical and photovoltaic applications. In the first case, the materials can be used as x-ray scintillators or x-ray storage phosphors, in the latter case as down-converting top layers for highly efficient solar cells. The glasses are based on a modified ZBLAN composition, i.e. a mixture of Zr, Ba, La, Al, and Na fluorides. They are additionally doped with chlorine ions to initiate the growth of $BaCl_2$ nanocrystals upon thermal processing. Eu^{2+} ions are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon ultraviolet or x-ray excitation. The nanocrystal size and structural phase depend significantly on the heating conditions and Eu doping level. X-ray diffraction patterns show a structural phase change of the $BaCl_2$ nanocrystals from hexagonal to orthorhombic as annealing temperatures are increased. DSC experiments were performed to obtain activation energies, thermal stability parameters and information on the crystal growth mechanisms.

DF 18.9 Thu 11:45 H38

Time-resolved optical spectroscopy on Er-doped fluorozirconate-based glasses for efficient up-conversion — •Ulrich Skrzypczak[1], Manuela Miclea[1], Jacqueline A. Johnson[2], and Stefan Schweizer[1,3] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Department of Materials Science and Engineering, University of Tennessee Space Institute, Tullahoma, TN 37388, USA — [3]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale)

Fluorozirconate(FZ)-based glasses have shown their potential as hosts for rare-earth (RE) ions such as Er, in these glasses REs show emissions that would be quenched in other glasses. Such material systems are of practical interest for photon up-conversion. For photovoltaic applications, the efficiency of bifacial solar cells could be vastly improved by an up-converting back layer. Up-conversion is the sequential absorption of two or more low-energy infrared photons by a RE ion followed by subsequent emission of a visible photon. This process is dependent on the intermediate level lifetime of the RE ion, which is determined by the phonon energies of the host material. Low phonon energy glasses like FZ glasses are thus desirable hosts. The lifetimes of the energy levels involved in the up-conversion process are investigated by time-resolved spectroscopy. Short laser pulses at different wavelengths are used for excitation; the emissions are detected via time-correlated photon counting. The radiative and non-radiative decay processes in Er-doped FZ glasses are analyzed and discussed.

DF 18.10 Thu 12:00 H38

Spectral down-conversion in Sm-doped borate glasses for photovoltaic applications — •Marcel Dyrba[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Samarium fluorescence in glasses has attracted much attention in the past two decades, in particular for studies on spectral-hole burning, excited state absorption, and laser properties. Here, a class of Sm-doped borate glasses has been developed for photovoltaic applications. The fluorescent glass is placed on top of a solar cell and, in the case of Sm^{3+} doping, converts the incident violet/blue part of the solar spectrum to red light which is more efficiently absorbed by the solar cell. The chemical base composition of borate glasses consists of the network former boron oxide and metal oxides as network modifiers. The spectroscopic properties of Sm^{3+}, in particular the fluorescence efficiency, are significantly influenced by the electron negativity of the network modifier. Some of the glasses are additionally doped with silver oxide. Subsequent heat treatment causes reduction of the doped silver ions and leads to the formation of metallic silver nanoparticles. The effect of the local field enhancement around the Sm^{3+} ions, which is due to surface plasmons from the silver nanoparticles being close by, is investigated.

DF 18.11 Thu 12:15 H38

Raman spectroscopy on barium halide nanoparticles in fluorozirconate-based glasses — •Charlotte Pfau[1], Paul-Tiberiu Miclea[2,3], and Stefan Schweizer[1,2] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

Rare-earth(RE) doped fluorozirconate-based glasses show enhanced fluorescence properties when they are additionally doped with Cl or Br ions, which initiate the growth of $BaCl_2$ or $BaBr_2$ nanocrystals, respectively, upon thermal processing. The REs are incorporated into the nanocrystals during the annealing procedure enabling a strong fluorescence upon excitation. A critical parameter for the fluorescence efficiency is the non-radiative decay process from the excited to the ground state. Non-radiative decay processes are determined by the phonon energies of the host system. Low phonon energy systems such as $BaCl_2$ or $BaBr_2$ are desirable hosts for fluorescent ions. The size and structural phase of the nanocrystals depend significantly on the heating conditions; consequently, a series of chlorine- or bromine-doped fluorozirconate-based glasses were analyzed to determine their phonon energy spectra by Raman spectroscopy. For comparison, the phonon spectra of bulk $BaCl_2$, and $BaBr_2$ were investigated.