Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks and Sessions

(lecture rooms ER 164, EB 107 and EB 407; Poster G)

Invited Talks

DF 2.1	Mon	10:00–10:40	EB 107	**Recent Progress in Polymeric LED** — •Klaus Meerholz
DF 4.1	Mon	14:00–14:40	EB 107	**High-k gate dielectrics on silicon and on high-mobility semiconductors: Atomic-scale phenomena underlying transistor performance** — •Martin M. Frank
DF 5.1	Mon	14:30–15:10	EB 407	**Behaviour of Ferroelectrics Influenced by Nanoscale Morphology** — •john martin gregg, alina schilling, liwu chang, mark mcmillen, mohamed saad, robert bowman, gustau catalan, james scott, finlay morrison
DF 6.1	Tue	9:30–10:00	EB 407	**Glass freezing in confined geometries studied by DMA** — •Wilfried Schranz, Johannes Koppensteiner, Madalina-Roxana Puica
DF 7.1	Tue	10:00–10:40	EB 107	**Modelling of Point Defects in Ferroelectric Materials** — •Karsten Albe, Paul Erhart
DF 7.2	Tue	10:40–11:20	EB 107	**Polarons in lithium niobate** — •Ortwin Schirmer
DF 12.1	Thu	10:00–10:40	EB 107	**Piezoelectric ceramic materials - a success story** — •Dieter Sporn, Andreas Schönecker, Bernhard Brunner, Horst Beige

Tutorial "Basics of polar oxides"

DF 1.1	Sun	14:00–15:30	ER 164	**Physik der Ferroelektrika - Grundlagen** — •Christoph Buchal
DF 1.2	Sun	15:30–17:00	ER 164	**Ferroelektrische Schichten und Heterostrukturen** — •Hermann Kohlstedt

Internal symposium "High-k dielectrics for highly scaled Silicon-based Micro- and Nanoelectronics"

Organisation: Th. Schroeder, IHP-Microelectronics, Frankfurt/Oder

DF 4.1	Mon	14:00–14:40	EB 107	**High-k gate dielectrics on silicon and on high-mobility semiconductors: Atomic-scale phenomena underlying transistor performance** — •Martin M. Frank
DF 4.2	Mon	14:40–15:05	EB 107	**Molecular Beam Epitaxy of crystalline oxides on Si for C-MOS and for the monolithic integration of semiconductors on Silicon** — •Saint-Girons Guillaume, Merckling Clément, El-Kazzi Mario, Becerra Loic, Regreny Philippe, Patriarche Gilles, Largeau Ludovic, Favre-Nicolin Vincent, Hollinger Guy
DF 4.3	Mon	15:05–15:30	EB 107	**Damascene metal gate technology: A solution to high-k gate stack challenges?** — •Udo Schwalke
DF 4.4	Mon	15:30–16:10	EB 107	**Do new materials solve the upcoming challenges of future DRAM memory cells?** — •Uwe Schröder
DF 4.5	Mon	16:10–16:35	EB 107	**AVD and ALD developments for next generation MIM capacitors and memory applications** — Peter K. Baumann, Christoph Lohe, •Michael Heuken

DF 4.6	Mon	16:35–17:00	EB 107	**MIM Capacitors for Wireless Communication Technologies** — •Christian Wenger

Internal symposium "Point defect spectroscopy and engeneering"

Organisation: R. Eichel, Technische Universität Darmstadt

DF 7.1	Tue	10:00–10:40	EB 107	**Modelling of Point Defects in Ferroelectric Materials** — •Karsten Albe, Paul Erhart
DF 7.2	Tue	10:40–11:20	EB 107	**Polarons in lithium niobate** — •Ortwin Schirmer
DF 7.3	Tue	11:20–11:40	EB 107	**Local structure and symmetry of paramagnetic ions in microscopic and nanoscopic ferroelectric materials** — •Emre Erdem, Kamil Kiraz, Mehmet Somer, Rüdiger -A. Eichel
DF 7.4	Tue	11:40–12:00	EB 107	**The effect of (Gd^{3+},Cu^{2+}) and (Gd^{3+},Fe^{3+}) Co-Doping on the Defect Chemistry of $PbTiO_3$** — •Michael Drahus, Rüdiger Eichel, Emre Erdem, Hans Kungl, Michael Hoffman
DF 7.5	Tue	12:00–12:20	EB 107	**Influence of extrinsic defects on the recombination behavior of light-induced hole and electron polarons in $KNbO_3$** — •Bettina Schoke, Christoph Merschjann, Stefan Torbrügge, Mirco Imlau
DF 7.6	Tue	12:20–12:40	EB 107	**Solid-state NMR on defects in lead titanates** — •Marko Bertmer, Rüdiger Eichel, Hans Kungl
DF 7.7	Tue	12:40–13:00	EB 107	**Gitterplatzbestimmung und Ausheilverhalten von Hf implantiertem CaF_2** — •Thomas Geruschke, Reiner Vianden

Invited talks of the joint symposium SYNF

See SYNF for the full program of the Symposium.

Invited talks of the joint symposium SYEC

See SYEC for the full program of the Symposium.

Sessions

DF 1.1–1.2	Sun	14:00–17:00	ER 164	**Tutorial: Basics of Polar Oxides**
DF 2.1–2.8	Mon	10:00–13:00	EB 107	**Electric, electromechanical and optical properties I**
DF 3.1–3.5	Mon	10:40–12:20	EB 407	**Phase Transitions**
DF 4.1–4.6	Mon	14:00–17:00	EB 107	**High-k dielectrics for highly scaled Silicon-based Micro- and Nanoelectronics**
DF 5.1–5.8	Mon	14:30–17:30	EB 407	**Scanning and diffraction methods**
DF 6.1–6.10	Tue	9:30–12:15	EB 407	**Glasses I (joint session DF/DY)**
DF 7.1–7.7	Tue	10:00–13:00	EB 107	**Point defect spectroscopy and engeneering**
DF 8.1–8.7	Tue	14:30–16:15	EB 407	**Glasses II (joint session DF/DY)**
DF 9.1–9.19	Tue	15:00–18:00	Poster G	**Poster**
DF 10.1–10.7	Wed	14:30–16:15	EB 407	**Glasses III (joint session DF/DY)**
DF 11.1–11.9	Wed	14:00–17:00	EB 107	**Dielectric and ferroelectric thin films and nanostructures I**
DF 12.1–12.8	Thu	10:00–13:00	EB 107	**Dielectric and ferroelectric thin films and nanostructures II**
DF 13.1–13.9	Thu	14:00–17:00	EB 107	**Dielectric and ferroelectric thin films and nanostructures III**
DF 14.1–14.10	Thu	14:00–17:20	EB 407	**Electric, electromechanical and optical properties II**

Annual General Meeting of the Dielectric Solids Division

Mittwoch 17:30–18:30 Raum EB 107

- Bericht des Fachverbandsleiters
- Tagungsnachlese
- Eingeladene Vorträge für 2009
- Fachinterne und fachübergreifende Symposia 2009
- Verschiedenes

DF 1: Tutorial: Basics of Polar Oxides

Time: Sunday 14:00–17:00 Location: ER 164

Tutorial DF 1.1 Sun 14:00 ER 164

Physik der Ferroelektrika - Grundlagen — •Christoph Buchal — Institut für Bio- und Nanosysteme (IBN1-IT), Forschungszentrum Jülich, 52425 Jülich

Ferroelektrika sind eine physikalisch und technisch hoch interessante Materialklasse. Wir betrachten, wie sich die ferroelektrischen Eigenschaften aus den atomaren Anordnungen in den Kristallstrukturen ergeben und wie sich Ferroelektrika in charakteristischer Weise von Ferromagneten unterscheiden. Dazu erläutern wir wichtige Beispiele von einkristallinen und polykristallinen Materialien und diskutieren ihre elektrischen, optischen, mechanischen und thermischen Eigenschaften und ihre wechselseitigen Kopplungen. Als wichtige optische Anwendungen werden verschiedene Modulatoren und holographische Speicher erklärt.

Tutorial DF 1.2 Sun 15:30 ER 164

Ferroelektrische Schichten und Heterostrukturen — •Hermann Kohlstedt — Forschungszentrum Jülich, Institut für Festkörperforschung, 52425 Jülich

Dünne ferroelektrische Schichten werden erfolgreich in vielen Gebieten der modernen Mikro- und Nanoelektronik eingesetzt. Einführend werden die wesentlichen Depositionsmethoden dünner ferroelektrischer Schichten erklärt. Hierzu gehört das Sputtern, die Pulsed Laser Deposition, die Molekularstrahlepitaxie und die metall-organische Gasphasen- Deposition. Stellvertretend für die Anwendung ferroelektrischer Schichten werden das FeRAM (Ferroelectric Random Access Memory) und der ferroelektrische Feldeffekttransistor als nichtflüchtige Speicherbauelemente beschrieben. Dabei wird auf die physikalischen Prinzipen, die Schaltungstechnik sowie mögliche Fehlermechanismen, wie Fatigue, Imprint und Retention eingegangen. Das Tutorial schließt mit einem Abriss über aktuelle Fragestellungen im Bereich ferroelektrischer Heterostrukturen. Skalierungseffekte in ultradünnen Schichten und die Physik polarer Grenzflächen stehen dabei im Mittelpunkt. Anhand von ausgewählten Beispielen wird demonstriert, wie erfolgreich und viel versprechend das "Interface und Strain Engineering" als Wechselspiel zwischen Filmdeposition, der Anwendung modernster analytischer Verfahren sowie die Umsetzung in Bauelemente ist. Ferroelektrische Bauelemente, in denen eine einzige Atomlage die wesentlichen Eigenschaften bestimmt sind denkbar. Jetzt schon ist absehbar, dass diese attraktiven Möglichkeiten neue Zielrichtungen für Bauelemente und in der Grundlagenforschung eröffnen wird.

DF 2: Electric, electromechanical and optical properties I

Time: Monday 10:00–13:00 Location: EB 107

Invited Talk DF 2.1 Mon 10:00 EB 107

Recent Progress in Polymeric LED — •Klaus Meerholz — Physikalische Chemie, Universität Köln, Luxemburgerstr. 116, 50939 Köln

Organic light emitting diodes (OLEDs) based on electroluminescent conjugated polymers are considered as a promising alternative for display and lighting applications, mainly due to their better compatibility with low-cost production techniques and large substrates. A challenge is multiple-layer deposition to improve the efficiency of the devices and, as a result, their lifetime.

This contribution summarizes recent trends in the field of OLED with an emphasis on solution-processed devices. We have in the past developed photochemically crosslinkable semiconductors for fabrication of complex multilayer OLED with a potential for eventually becoming organic lasers and RGB-pixelation [1-2].

[1] C.D. Müller, A. Falcou, N. Reckefuss, M. Rojahn, V. Wiederhirn, P. Rudati, H. Frohne, O. Nuyken, H. Becker, K. Meerholz, Nature 421, 829 (2003). [2] M.C. Gather, A. Köhnen, A. Falcou, H. Becker, Klaus Meerholz, Adv. Funct. Mat. 17, 191 (2007).

DF 2.2 Mon 10:40 EB 107

Molecular hybrids for optical switching — •Andrea Schuy, Theo Woike, and Dominik Schaniel — 1. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln

$(CN_3H_6)_2Fe(CN)_5NO$ (guanidinium nitroprusside = GuNP) has the ability to form metastable isomers with a change of refractive index after irradiation with laser light in the blue-green spectral range. One isomer is formed by a rotation of the NO ligand around 180° to turn the Fe-NO into a Fe-ON coordination. By subsequent irradiation with light in the near infrared spectral range the 180°-ligand rotates around 90° to a side-on position [1]. This ability remains unaffected after embedding $(CN_3H_6)_2Fe(CN)_5NO$ into a silica-gel matrix, even down to dilution to single-molecules. We investigated differences between the behavior of the crystalline GuNP and GuNP embedded in gel due to the effects of complex-complex interactions and complex-matrix interactions respectively on the NO-vibration.

[1] D. Schaniel, M. Imlau, Th. Weisemoeller, Th. Woike, K. Krämer, H. U. Güdel; *Photoinduced nitrosyl linkage isomers uncover a variety of unconventional photorefractive media*; *Adv. Mat.* **19** (5), 723-726 (2007).

DF 2.3 Mon 11:00 EB 107

Hybrid Elastomers with Improved Electromechnical Properities — Torsten Finnberg and •Bernd-Joachim Jungnickel — Deutsches Kunststoff-Institut, Darmstadt, Germany

Dielectric elastomers are a promising material for solid-state actuators due to the high energy density which can be stored, the short response times, and the high obtainable strain. That strain is based on the Maxwell effect. It has the same electric field dependence as electrostriction but is ruled by the ratio between dielectric permittivity and Youngs modulus of the material. A technologically feasible route to optimise the electro-mechanical performance of a dielectric elastomer is consequently to increase its dielectric constant by blending with a high dielectric constant filler without simultaneous increase in stiffness. In doing that, hybrids of polydimethylsiloxane filled with nano-scaled titanium dioxide were prepared. The influence of the filler content on the mechanical, dielectric, and electro-mechanical behaviour was investigated. The dielectric constant increased linearly with filler contents up to 10 wt-%. On the other hand, the elastic modulus of the hybrids decreased slightly in that composition range. The electromechanical coupling coefficient exhibited consequently a maximum for a filler level of 6 wt-% where it increased by 140 % with respect to that of the unfilled material. The approach enables to tune the mechanical and electro-mechanical properties of a dielectric elastomer to a desired ratio.

DF 2.4 Mon 11:20 EB 107

Time- and frequency-domain polarization imaging on poly(vinylidenefluoride-co-trifluoroethylene) films — •Rosaura Flores Suárez[1], Axel Mellinger[1], Werner Wirges[1], Reimund Gerhard[1], Cong-Duc Pham[2], Anca Petre[2], Laurent Berquez[2], and Didier Marty-Dessus[2] — [1]University of Potsdam, Department of Physics, 14469 Potsdam, Germany — [2]Paul Sabatier University, Laboratory on Plasma and Conversion of Energy, 31062 Toulouse, France

Three-dimensional tomography of space-charge and polarization distributions are of high interest for the electrical characterization of new dielectric materials. In this work, two non-destructive thermal methods called TPT (Thermal-Pulse Tomography) and FLIMM (Focused Laser-Intensity Modulation Method) are presented and compared. FLIMM is implemented in the frequency domain, while TPT works in the time domain. In an effort to further increase the lateral resolution while minimizing the thermal stress on the sample, 3D polarization images of poly(vinylidenefluoride-co-trifluoroethylene) (PVDF-TrFE) films poled with a well-defined grid-pattern electrode were obtained. The PVDF-TrFE (65%-35%) films (12 μm thickness) were prepared by means of drop casting. The 3D polarization maps show a polarization starting at a depth of 0.2 μm. In low- and high-resolution

scans, the details of the grid electrode are very well reproduced and non-uniformities of polarization along some arms are seen, respectively. These results will be compared with simulations taking into account the 3D heat flow.

DF 2.5 Mon 11:40 EB 107

Cellular polymer ferroelectrets for generation and detection of air-borne ultrasound — •Petr Bartu[1], Mario Dansachmüller[1], Ivan Minev[2], Ingrid Graz[2], Nikita Arnold[1], and Siegfried Bauer[1] — [1]Soft Matter Physics, Johannes Kepler University, Linz, Austria — [2]Nanoscience Centre, University of Cambridge, UK

Charged cellular polypropylene ferroelectrets can be used as sensors and transducers in many applications (e.g. pressure measurements, microphones and loudspeakers). The suitability of different materials for generating and detecting air-borne ultrasound can be compared by means of a figure of merit (fom) $F = k^4/Z^2$, where k and Z denote the materials longitudinal coupling factor and acoustic impedance respectively. By comparison with piezoelectric ceramics and ferroelectric polymers, soft cellular foams possess the largest fom F.

In order to demonstrate the coupling quality of cellular ferroelectrets to air, samples of charged cellular polypropylene are investigated in an acoustical interferometer arrangement in a transmitting as well as in a reflecting mode. Due to the good coupling to air, Fabry-Perot resonances are observed together with the electromechanical thickness extension resonance of the cellular ferroelectret foam. Using a plane wave acoustical model, the observed Fabry-Perot resonances are confirmed and a straightforward derivation of the fom F is presented. Work partially supported by the FWF.

DF 2.6 Mon 12:00 EB 107

Flexible Touch- and Pressure Sensitive Piezo Elastomer Stretch Sensor for Simple Surface Point Location Detection. — •Reinhard Schwödiauer, Christoph Orthwein, Gerda Buchberger, Ingrid Graz, Petr Bathu, and Siegfried Bauer — Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria

Mechanical flexibility is a central advantage and an auspicious goal for the branch of macroelectronics, dealing with the development of plastic electronic products and related sensors. In many application fields however, flexibility alone is not sufficient: Examples include technical skin-sensors for robotics or wearable, fabric-integrated large-area sensors. Sensors and actuators in such application fields should be stretchable and not just flexible. Therefore, the development of flexible, touch sensitive sensors is a challenging task in plastic electronics.

We present simple designs for large-area elastomeric touch- and pressure sensors based on cellular polypropylene ferroelectrets in combination with conductive poly(dimethylsilicone). Both the preparation, the morphological characterization as well as the performance of the sensor is discussed. In addition a simple concept is introduced, allowing for spatially localizing single touch events. No complex structured array sensors are required, instead a nonstructured large area ferroelectret is used with electronic elements at the periphery of the device. A simple one-dimensional model is given to elucidate the concept. Experimetal results are used to illustrate the performance of the flexible and stretchable sensor systems.

DF 2.7 Mon 12:20 EB 107

Second Harmonic Generation an ungeordneten, porösen Materialien — •Susanne Lisinski[1], Dominik Schaniel[2], Lorenz Ratke[1] und Theo Woike[2] — [1]DLR, Institut für Materialphysik im Weltraum, Köln, Deutschland — [2]Universität zu Köln, 1. Physikalisches Institut, Köln, Deutschland

Im Rahmen dieser Arbeiten werden ferroelektrische $LiTaO_3$ und $LiNbO_3$ Xerogele mittels eines Sol-Gel Verfahrens synthetisiert und auf ihre frequenzverdoppelnden Eigenschaften untersucht. Die hergestellten Materialien bestehen aus einem Netzwerk ungeordneter, ferroelektrischer Kristallite mit einem einstellbaren Kristallitdurchmessers von 100 nm-3 μm. Second Harmonic Generation (SHG) der porösen Materialien wird mit Hilfe eines gepulsten Nd:YAG Lasers mit einer Wellenlänge von λ_e=1064 nm erzeugt. Die generierte Strahlung ist aufgrund der ungeordneten polaren Achsen der Kristallite diffus. In diesem Vortrag wird die Sol-Gel-Synthese und Charakterisierung der Materialien, wie auch die Abhängigkeit der SHG-Energie von der Probendicke, Kristallitgrösse und Stöchiometrie, vorgestellt.

DF 2.8 Mon 12:40 EB 107

Dynamics of optical degradation on LiB_3O_5-crystal surfaces during SFG — •Stefan Möller, Änne Andresen, and Mirco Imlau — Department of Physics, University of Osnabrück, D-49069 Osnabrück

We have investigated the phenomenon of optical degradation of LiB_3O_5 single crystal surfaces during sum-frequency generation (SFG) of UV-light (λ = 355 nm) by a focused Q-switched Nd:YAG laser (f = 20 kHz, τ_{1064} = 10 ns, $\overline{P}_{1064}$ = 1.5 W). The investigations were performed on timescales > 100 h and UV-intensities below the light induced damage threshold of the crystals. The degradations were studied with optical and analytical methods.

As a result we found a steady deposition of foreign material on the output crystal surface in the illuminated area. Here, XPS uncovered several foreign elements as Na, S, Si, Ca, C beside B and O depending on the composition of the ambient atmosphere during SFG. The temporal development of the degradation could be observed by measuring the beam profile behind the crystal. The beam divergence increased as a function of the deposition height, which led to a complex intensity profile in the far-field. Further illuminating lead to a catastrophic break-down of the surface and the beam profile. This is due to thermal damage originating from the UV-absorption of the deposited material. Three models for the deposition process are discussed: a) diffusion out of the LiB_3O_5-subsurface, b) deposition of atoms of the ambient atmosphere, c) chemical reactions of LiB_3O_5, water, and boric acid. Financial support by the DFG (TFB 13, project A5/13-04).

DF 3: Phase Transitions

Time: Monday 10:40–12:20 Location: EB 407

DF 3.1 Mon 10:40 EB 407

Temperature-driven structural transformations in relaxor-ferroelectric $PbSc_{0.5}Ta_{0.5}O_3$ and $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ — Boriana Mihailova[1], •Bernd Maier[1], Carsten Paulmann[1], Thomas Malcherek[1], Jörg Ihringer[2], Martin Gospodinov[3], Rainer Stosch[4], Bernd Güttler[4], and Ulrich Bismayer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Universität Tübingen, Tübingen, Germany — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

X-ray diffraction and Raman spectroscopic studies in a wide temperature range on perovskite-type relaxors $PbSc_{0.5}Ta_{0.5}O_3$ (PST) and $Pb_{0.78}Ba_{0.22}Sc_{0.5}Ta_{0.5}O_3$ (PBST) are presented. The temperature evolution of phonon anomalies and the pseudo-cubic unit cell parameter for both PST and PBST reveals the existence of a critical temperature T^* between the Burns temperature T_B and the temperature of the dielectric-permittivity maximum T_m. T^* is associated with coupling of initially nucleated polar sub-clusters and their aggregation into larger polar nanoclusters. The temperature range between T_B and T^* is characterized by coupling between adjacent off-centered BO_6 octahedra to form initial polar clusters, while the range between T^* and T_m is characterized by coupling between off-centered B-cations from adjacent polar clusters. Off-centered Pb atoms exist even above T_B and their coherence length governs the coupling between polar regions comprising B-cation off-centered shifts and directs the formation of proper or relaxor ferroelectric state.

DF 3.2 Mon 11:00 EB 407

Transformation from ferroelectric to relaxor state in $BaTiO_3$ based relaxor ferroelectrics — •Vladimir Shvartsman[1], Wolfgang Kleemann[1], Jan Dec[2], Sheng-Guo Lu[3], Zheng Kui Xu[3], and Jiwei Zhai[4] — [1]Angewandte Physik, Universität Duisburg-Essen. Duisburg, Germany — [2]Institute of Physics, University of Silesia, Katowice, Poland — [3]Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, China — [4]Functional Materrials Research Laboratory, Tongji University, Shanghai, China

Presently considerable interest is focused onto the investigation of environment-friendly lead-free relaxors, in particular those based on the ferroelectric $BaTiO_3$. In these materials relaxor properties are observed not only at heterovalent cation substitution as in most relaxors, but also at isovalent substitution. We report on results of investigations of $Ba(Ti_{1-x}Sn_x)O_3$ (BTSn) and $Ba(Ti_{1-x}Zr_x)O_3$ (BTZ), x=0.1-0.4, ceramics which show a gradual transformation from ferroelectric to relaxor behavior at decreasing titanium content. Low-frequency dielectric spectroscopy and piezoresponse force microscopy were applied in order to distinguish the ferroelectric and relaxor features. The ferroelectric state is evidenced in BTSn and BTZ with $x < 0.175$ and 0.25, respectively. The broadening of the peak of the dielectric permittivity ("diffuse phase transition") is due to the coexistence of ferroelectric domains and paraelectric regions related to a nanoscale compositional segregation into Ti-rich and Ti-depleted regions. Further decrease of Ti-content results in relaxor behavior, which is supposed to be related both to weak random fields and to disorder inherent in pure $BaTiO_3$.

DF 3.3 Mon 11:20 EB 407

Pressure-induced phase transition in $PbSc_{0.5}Ta_{0.5}O_3$ — Boriana Mihailova[1], Ross J. Angel[2], •Anna-Maria Welsch[1], Jing Zhao[2], Jens Engel[2], Carsten Paulmann[1], Mihail Gospodinov[3], Rainer Stosch[4], Bernd Güttler[4], and Ulrich Bismayer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Virginia Tech, Blacksburg, USA — [3]Institute of Solid State Physics, Sofia, Bulgaria — [4]PTB Braunschweig, Germany

Relaxors are ferroelectrics with peculiar structural and physical features having various technological applications. The relaxor structural state consists of polar nanoclusters incorporated into a paraelctric matrix. The temperature evolution of polar nanodomains has been extensively analyzed but up to now only few structural studies have been performed under high pressures.$PbSc_{0.5}Ta_{0.5}O_3$ (PST) is a model representative of Pb-based perovskite-type relaxors. High-pressure studies on PST are rather fruitful to give deeper insights on relaxor structure in general, because: (i) PST shows long-range compositional B-site cation ordering of variable degree; (ii) the temperature of dielectric-permitivitty maximum is near 280 K, suggesting well pronounced polar nanoclusters at room temperature. We report on pressure-induced structural transformations in single-crystal PST samples up to 10 GPa. The structural changes were followed by in-house and synchrotron single-crystal X-ray diffraction and Raman scattering. A continuous phase transition was revealed by the appearance of a soft mode, change in the volume compressibility, broadening of the diffraction maxima and suppression of the x-ray diffuse scattering.

DF 3.4 Mon 11:40 EB 407

Pressure-induced phase transitions in the multiferroic $BiFeO_3$ studied by infrared spectroscopy — •Alexej Pashkin[1], Kaneez Rabia[1], Simone Frank[1], Raphael Haumont[2], Jens Kreisel[3], and Christine A. Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, , 86159 Augsburg, Germany — [2]Laboratoire de Physico-Chimie de l'Etat Solide ICMMO - UMR CNRS, Université Paris Sud, 91405 Orsay Cedex, France — [3]Laboratoire des Matériaux et du Génie Physique (CNRS), INP Grenoble - MINATEC 38016 Grenoble, France

$BiFeO_3$ is considered to be one of the model multiferroic materials with unusually high temperatures of antiferromagnetic ($T_N \sim 370$ °C) and ferroelectric ($T_C \sim 830$ °C) ordering. Recently, an extremely high spontaneous polarization has been reported for $BiFeO_3$ thin films, ceramics and crystals making this material very attractive for applications. $BiFeO_3$ presents a complex interplay between the magnetic, ferroelectric and ferroelastic order parameters. Thus, a particularly rich phase diagram is expected for this material.

We report a high-pressure infrared spectroscopic study of high-quality $BiFeO_3$ single crystals in the far-infrared range up to 10 GPa. The observed behavior of the infrared phonon modes under pressure clearly reveals two structural phase transitions around 3.0 and 7.5 GPa supporting the results of recent Raman and x-ray diffraction studies under pressure. *Financially supported by the DFG (Emmy Noether-program, SFB 484). Provision of beamtime at the ANKA (Karlsruhe) is acknowledged.*

DF 3.5 Mon 12:00 EB 407

Novel complexity in the phase diagram of ferroelectrics — •Annette Bussmann-Holder[1], Helmut Büttner[2], and Alan R. Bishop[3] — [1]Max-Planck-Institut Für Festköroerforschung, Heisenbergstr.1, D-70569 Stuttgart, Deutschland — [2]Lehrstuhl für Theoretische Physik, Universität Bayreuth, Bayreuth, Deutschland — [3]Los Alamos National Laboratory, Los Alamos, NM 87545, USA

The temperature/ doping dependent phase diagram of ferroelectric perovskite oxides is shown to be characterized by six different temperature scales: At high temperatures a crossover from paraelectric to paraelectric / ferroelastic behavior sets in followed by the onset of fluctuating ferroelastic clusters with doping and temperature dependent size. The cluster size anti correlates with their volume which defines another transition line. The onset of ferroelectricity is not sharp since para- and ferroelectric solutions coexist in a small temperature regime. The ferroelectric phase shows novel effects since from a certain transition temperature on this state is incomplete, i.e., ferroelastic clusters fluctuate in a polar matrix. Finally ferroelectricity is completely suppressed by quantum fluctuations. In addition, a novel phenomenon is discussed, where it is shown that the ferroelectric soft modes controls preceding structural instabilities

DF 4: High-k dielectrics for highly scaled Silicon-based Micro- and Nanoelectronics

Time: Monday 14:00–17:00 Location: EB 107

Invited Talk DF 4.1 Mon 14:00 EB 107

High-k gate dielectrics on silicon and on high-mobility semiconductors: Atomic-scale phenomena underlying transistor performance — •Martin M. Frank — IBM T.J. Watson Research Center, 1101 Kitchawan Road, Yorktown Heights, NY 10598, USA

Computer chip technology is undergoing a materials revolution: Hafnium-based high-permittivity ('high-k') dielectrics are replacing the silicon oxide gate insulator in metal-oxide-semiconductor field-effect transistors (MOSFETs); and metals are replacing the polycrystalline silicon gate electrode. These changes allow us to extend the exponential increase in integration density and performance known as Moore's Law. Researchers are even attempting to replace the silicon channel itself by high-carrier-mobility semiconductors, such as germanium, III-V compounds, carbon nanotubes, or graphene.

I will provide an overview of the materials science underlying MOSFET performance. First, properties and scaling of the traditional silicon oxide insulator will be summarized. Then, focus will be on non-epitaxial Hf-, Al-, and Ti-based dielectrics on silicon and on high-mobility semiconductors. We describe how processing parameters determine stack structure, e.g. continuity of the high-k layer, interface composition, and oxygen vacancy concentration. Comparing Si to Ge and III-V substrates, differences in interface formation will be rationalized based on thermodynamic considerations. Finally, we illustrate how the stack structure determines device characteristics such as gate leakage, gate stack capacitance, threshold voltage, and carrier mobility.

Invited Talk DF 4.2 Mon 14:40 EB 107

Molecular Beam Epitaxy of crystalline oxides on Si for C-MOS and for the monolithic integration of semiconductors on Silicon — •Saint-Girons Guillaume[1], Merckling Clément[1], El-Kazzi Mario[1], Becerra Loic[1], Regreny Philippe[1], Patriarche Gilles[2], Largeau Ludovic[2], Favre-Nicolin Vincent[3], and Hollinger Guy[1] — [1]INL/UMR5270-Site ECL, 36 av Guy de Collongue, 69134 Ecully cedex, France — [2]LPN UPR20/CNRS Route de Nozay, 91460 Marcoussis cedex — [3]cCEA/DRFMC/SP2M, 17 rue des Martyrs 38054 Grenoble and UJF, BP53, 38041 Grenoble cedex 9, France

In this contribution, a detailed description of the growth mechanisms and structural properties of high-k Al_2O_3, Gd_2O_3 and amorphous $LaAlO_3$ on Si will be presented. On the basis of these studies, relevant oxide/Si systems will be proposed that fulfill the requirements of future C-MOS systems. In particular, very promising electrical characteristics have been obtained showing that the (amorphous $LaAlO_3$)/Si system is compatible with ITRS recommendations in terms of EOT and leakage current. Moreover, it will also be shown that InP/oxide heterointerfaces present a quasi-ideal compliant behavior that opens

the way to the monolithic integration of III-V heterostructures on Si for advanced micro and optoelectronic applications.

Invited Talk DF 4.3 Mon 15:05 EB 107

Damascene metal gate technology: A solution to high-k gate stack challenges? — •Udo Schwalke — Darmstadt University of Technology, Darmstadt, Germany

Since the late 1960s, the normal fabrication method of CMOS transistors is known as the "gate first" approach. As the name indicates, gate dielectric and gate electrode are made first, i.e. prior to the self-aligned formation of the source (S) and drain (D) junctions by ion-implantation. As long as the gate stack has been made out of polycrystalline silicon and silicon dioxide, process integration was not an issue. Both materials are able to withstand high annealing temperatures and are compatible with reactive ion etching. However, after introducing novel gate stack materials, like high-k gate dielectrics and metal gate electrodes, the situation has been changed completely. These new materials are sensitive and degrade during high-temperature processing. In order to circumvent process-induced gate-stack damage, we have developed a "gate last" process flow, in which the self-aligned gate stack is made after S/D junctions. For the first time, fully functional metal gate MOSFETs with crystalline high-k dielectric have been fabricated by means of chemical mechanical polishing (CMP). Electrical results and details of the "gentle" damascene metal gate technology will be presented. To which extent the "gate last" approach is a general solution to the high-k metal gate challenges will be discussed.

Invited Talk DF 4.4 Mon 15:30 EB 107

Do new materials solve the upcoming challenges of future DRAM memory cells? — •Uwe Schröder — Qimonda Dresden GmbH & Co. OHG, Koengisbruecker Strasse 180, 01099 Dresden

A permanent trend in miniaturization of semiconductor DRAM devices has required continuous introduction of new materials. Specially, for capacitor and transistor applications a strong push for new dielectric materials and metal electrodes is ongoing. As design rules for capacitors are dropping below 50nm geometrical options turn out to be more and more challenging. Dielectrics with permittivity values more than 30 and metal electrodes become important. In the past few years the introduction of AlO-, HfO-, and ZrO-based dielectric materials with TiN electrodes were reported. The main focus of this work is to compare mixed and laminate dielectric films in terms of crystallographic phase resulting in capacitance enhancement and leakage current improvement. Optimized dielectric properties were reached for doped HfO- and ZrO dielectrics in a cubic/ tetragonal phase. Simultaneously, conventional SiON/Poly-Si gate devices will be replaced by high-k dielectric/metal gate structures for continuous scaling. Here industry narrowed down the choice of high-k dielectrics to HfO-based materials. Depending on the device specifications different metal electrodes are proposed. Trends, progress, and challenges will be reviewed.

Invited Talk DF 4.5 Mon 16:10 EB 107

AVD and ALD developments for next generation MIM capacitors and memory applications — Peter K. Baumann, Christoph Lohe, and •Michael Heuken — AIXTRON AG, Aachen, Germany

Atomic layer deposition (ALD) enables deposition of electrode, dielectric and barrier layers on high aspect ratio trench structures and has been widely used. However, due to its nature the throughput is typically limited. Atomic vapor deposition (AVD®) is a special type of metal organic vapor deposition (MOCVD) that enables deposition with high precursor gas phase saturation. This results in improved throughput while maintaining conformal deposition on moderate aspect ratio trench structures. Based on the International Roadmap for Semiconductors (ITRS) for front end, for DRAM at the 50nm and below technology node metal-insulator-metal (MIM) structures will be required [1]. Also conformal step coverage on structures with aspect ratios of 1:60 and higher as well as an equivalent oxide thickness (EOT) of less than 1nm will be necessary. Other memory applications (e.g. phase change memory) require less advanced aspect ratios, opening possibilities for AVD®. ALD and AVD® have been used to deposit electrode and dielectric films based on e.g. TiN, Ru, TaSiN as well as HfO_2, ZrO_2, Al_2O_3. Results for the different deposition techniques and various process conditions will be presented and compared considering use for memory applications.

[1] Front end, International Roadmap for Semiconductors (Semiconductor Industry Association, Palo Alto 2006 update).

Invited Talk DF 4.6 Mon 16:35 EB 107

MIM Capacitors for Wireless Communication Technologies — •Christian Wenger — IHP, Im Technologiepark 25, 15236 Frankfurt Oder

The high-k Metal-Insulator-Metal (MIM) capacitor BEOL integration into circuits for wireless communication is characterized by the efforts toward increasing the capacitance density, reducing the leakage current density and improving the voltage linearity. In particular, the achievement of sufficient capacitance voltage linearity in high-k MIM capacitors is still a challenge. Based on fundamental physical effects, the origin of the quadratic voltage dependence of high-k MIM capacitors will be presented.

DF 5: Scanning and diffraction methods

Time: Monday 14:30–17:30 Location: EB 407

Invited Talk DF 5.1 Mon 14:30 EB 407

Behaviour of Ferroelectrics Influenced by Nanoscale Morphology — •John Martin Gregg[1], Alina Schilling[1], Liwu Chang[1], Mark McMillen[1], Mohamed Saad[1], Robert Bowman[1], Gustau Catalan[2], James Scott[2], and Finlay Morrison[3] — [1]School of Maths and Physics, Queen's University Belfast, Belfast, U. K. — [2]Department of Earth Sciences, Cambridge University, Cambridge, UK — [3]Department of Chemistry, University of St Andrews, St Andrews, Scotland, U. K.

This talk describes attempts made to simplify the study of nanoscale ferroelectrics by minimizing the influence of defects, microstructure and to some extent boundary-related strain effects by using a Focused Ion Beam Microscope (FIB) to cut thin film sheets and nanowires directly from bulk single crystal ferroelectrics.

Low field permittivity characteristics of FIB-cut thin film $BaTiO_3$ sheets have been investigated, and it has been shown that bulk-like permittivity response persists even in films as thin as $\sim$70nm. This result contradicts decades of previous work done on conventionally grown thin film ferroelectric heterostructures.

In addition the domain characteristics of single crystal thin sheets and nanowires have been characterised as a function of scale and of morphology using Scanning Transmission Electron Microscopy. The domain periodicities and polar orientations observed show a dramatic sensitivity to both size and shape. It has been shown that nanoscale morphology can be used to control polar orientation along the lengths of single nanowires.

DF 5.2 Mon 15:10 EB 407

Fourier analysis of ferroelectric polarization reversal — •Andreas Rüdiger — Institute of Solid State Research, Research Center Jülich, Germany

The detection of nanoscale piezoelectricity is generally achieved by means of lock-in techniques. As the excitation voltage exceeds the coercive field, polarization reversal occurs with a complex fourier spectrum that contains information on the piezoelectric response, the electrostriction and the polarization reversal process. A quantitative spectral analysis in comparison to experimental data shows the potential of the method to cover the dynamic range from cantilever to domain wall dynamics.

DF 5.3 Mon 15:30 EB 407

Complete reconstruction of the piezoelectric tensor in $BaTiO_3$ nanoislands — •Sebastian Albiez, Serge Röhrig, and Andreas Rüdiger — Institut für Festkörperfosrschung, Forschungszentrum Jülich, 52425 Jülich

Due to the advancing miniaturization of non-volatile ferroelectric memories, a better separation of extrinsic and intrinsic contributions becomes mandatory. Piezoresponse force microscopy (PFM) is

the favored tool to investigate these phenomena as the third rank-piezoelectric tensor represents the crystallographic structure of the system and thus also allows for the discussion of the polarization. Current PFM systems achieve lateral resolutions of a few nanometers. The piezoelectric tensor describes the three-dimensional displacement of the tip in contact with the surface i.e. three linearly independent orthogonal forces on the tip. The optical lever arm method however only detects a lateral and a vertical displacement the latter one containing the information of vertical bending and vertical buckling while the first one only contains the information of lateral torsion. To disentangle these contributions a 90-degree rotation of the sample underneath the tip is required without losing the area under investigation. We present current experimental data on ferroelectric nanoislands and discuss them in terms of a complete reconstruction of the piezoelectric tensor where all three displacement modes of the cantilever are differentiated.

DF 5.4 Mon 15:50 EB 407

Electromechanical force microscopy as a non-destructive detection of local inhomgeneities with nanoscale — •Serge Röhrig and Andreas Rüdiger — Institute of Solid Research, Research Center Jülich, Germany

Detection of crystallographic defects and inhomgeneities is typically achieved by either non-destructive light or sound scattering with a lateral resolution of the order of the used wavelength or in a destructive way with atomic resolution by means of e.g. TEM. We present a non-destructive approach based on a standard piezoresponse force microscope detecting the second harmonic of the excitation voltage i.e. the electrostrictive response with nanometer resolution. We use the lateral torsion of the cantilever to monitor displacements that stem from any reduction of radial symmetry underneath the tip. While a globally reduced radial symmetry e.g. due to orthorhombic symmetry of the sample generates an undetectable background, any local variation causes a torque on the cantilever that can be monitored without need for any piezoelectric activity. We demonstrate the feasibility of this technique that is generally applicable to all crystalline dielectrics on any lengthscale.

DF 5.5 Mon 16:10 EB 407

Growth of C_{60} islands on TiO_2(110) — •Felix Loske, Frank Ostendorf, Michael Reichling, and Angelika Kühnle — Department of Physics, University Osnabrück, Germany

We have investigated the interaction of C_{60} molecules with a dielectric substrate, namely rutile TiO_2(110). Non-contact atomic force microscopy was used to study the adsorption structure and surface mobility in situ at room temperature. At submonolayer coverage the molecules adsorb preferencially at substrate step edges. Upon increasing coverage, islands grow from the decorated step edges on the lower terraces in an island growth mode. Simultaneous imaging of the substrate's bridging oxygen rows and the C_{60} island structure revealed that the C_{60} molecules are arranging in a rhombic supercell, with the molecules lying centered in the troughs between the bridging oxygen rows of the substrate. Domain boundaries were determined to run parallel to the supercell's basis vectors and are characterized by a single strand of protruding C_{60} molecules along the junction.

DF 5.6 Mon 16:30 EB 407

Atomic scale evidence for faceting stabilization of a polar oxide — •Frank Ostendorf, Stefan Torbrügge, and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barabarastr. 7, 49090 Osnabrück

Polar metal oxide surfaces are of highest importance for various applications like catalysis, sensor technology and optoelectronic devices. In matters of industrial applications and merit these surfaces represent a research field of general scientific interest. With this study we corroborate new aspects in the basic understanding of one of the most prominent polar surfaces, namely zinc oxide (ZnO). With respect to nanoelectronic devices the surface properties of zinc oxide and zinc oxide compounds are of greatest importance. By highest resolution dynamic scanning force microscopy (SFM) operated in the non-contact mode (NC-AFM), we reveal the complex stabilization mechanism of polar zinc terminated ZnO(0001). The nanoscopic and atomic structures unveiled corroborate a model of stabilization via triangular structures. High temperature preparation (T > 1300 K) yields a novel phase with an additional stabilization by faceting in the form of highly ordered step arrays. The terraces between steps are partly covered with triangular reconstructions exhibiting exclusively {1010} nano-facets on step edges. The combination of both mechanisms allow a complete stabilization of the surface without involvement of adsorbates.

DF 5.7 Mon 16:50 EB 407

Phonon resonances in ferroelectrics probed with scattering scanning near-field optical microscopy (s-SNOM) using a free-electron laser — •Lukas Eng[1], Susanne Schneider[1], Stefan Grafström[1], Stephan Winnerl[2], and Manfred Helm[2] — [1]Institute of Applied Photophysics, TU Dresden — [2]Forschungszentrum Dresden-Rossendorf

s-SNOM is based on the interaction between an optically scattering nanoparticle (AFM tip) and a dielectric sample. The size of the scatterer defines the resolution of the microscope, which is on the order of a few nanometers. We use here sample-enhanced phonon resonances to study the local optical properties of such anisotropic ferroelectrics.

We present the spectroscopic near-field examination of optically anisotropic ferroelectrics, namely lithium niobate ($LiNbO_3$) [1] and barium titanate ($BaTiO_3$). In these samples we excite phonon resonances in the IR regime. As we need to tune the incident wavelength exactly to the sample resonance, we use a free-electron laser at the Forschungszentrum Dresden-Rossendorf as a precisely tunable light source in the IR with a wavelength range 4-200 μm. Furthermore, we show near-field images of ferroelectric domains of $BaTiO_3$ representing a purely anisotropic near-field contrast. We are presenting the first tunable IR near-field measurements on ferroelectric single crystals, which are furthermore in excellent accordance with recent calculations of optical anisotropy in such systems [2].

[1] S.C. Schneider et al., Appl. Phys. Lett. 90, 143101 (2007)
[2] S.C. Schneider et al., Phys. Rev. B 71, 115418 (2007).

DF 5.8 Mon 17:10 EB 407

Time-resolved X-ray diffraction studies of piezoelectric actuators — •Florian Rödl, Peter Wochner, Ralf Weigel, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Stuttgart, Germany

Piezoelectric materials play an important role in different applications ranging from nanoscale positioners to diesel engine fuel injectors. The internal structure of most devices is highly inhomogeneous and consists of stacks of ceramic layers with asymmetric electrode configurations. It is crucial to understand the structural response to the electrical excitation on the level of the individual grains especially in view of their highly inhomogeneous environment. One of the open questions is how does the local dynamic response of these materials influence the switching and fatigue behavior. Here we present an experimental strategy to perform real-time X-ray experiments on bulk PZT actuators during switching.

In this talk I will discuss the experimental setup we used at different synchrotron beamlines and first in-situ results. Depending on different parameters, like e.g. excitation profile, preloading and grain location, the dynamic response of the crystal lattice will be presented. A microbeam setup was used to study single grains.

DF 6: Glasses I (joint session DF/DY)

Time: Tuesday 9:30–12:15 Location: EB 407

Invited Talk DF 6.1 Tue 9:30 EB 407

Glass freezing in confined geometries studied by DMA — •Wilfried Schranz, Johannes Koppensteiner, and Madalina-Roxana Puica — Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria

Dynamics in confined surroundings appears in many fields, i.e. in chemistry, physics, biology, material science, etc. Using a dynamic mechanical analyser (DMA) we measured [1] the low frequency elastic response of the glass former salol confined in silica based nanoporous media of various pore sizes (2.5nm to 7.5 nm). In addition to the glass

transition of the bulk material of salol we find a second freezing process, showing up in the real and imaginary parts of the complex elastic response. This is explained by a radial distribution of Vogel-Fulcher temperatures inside the pores, an assumption which is consistent with recent computer simulations [2] showing an increase of the molecular relaxation time with decreasing distance from rough pore surfaces. The observed glass transition temperatures decrease with decreasing pore size. The mechanism of the glass transition reduction will be discussed. Acknowledgements: Support by the Austrian FWF (P19284-N20) and the University of Vienna (IK 1022-N) is gratefully acknowledged.

[1] W. Schranz, M.R. Puica, H. Kabelka and A.V. Kityk. Europhys. Lett. 79, 36003 (2007) [2] P. Scheidler, W. Kob and K. Binder, Europhys. Lett. 59, 701 (2002).

DF 6.2 Tue 10:00 EB 407

Confined glass formers in nanoporous materials studied by ^{31}P NMR — •Sabine Gradmann[1], Gilberte Dosseh[2], Christiane Alba Simionesco[2], and Ernst Rössler[1] — [1]Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Laboratoire de Chimie Physique, CNRS-UMR 8000, Bâtiment 349, Université de Paris-Sud, 91405 Orsay, France

We investigate the dynamics of the glass former m-tricresylphosphate (mTCP) confined in the nanoporous matrices CPG, SBA15, MCM41 with different pore sizes, varying in diameter from 4nm up to 300nm, within a temperature range above the glass transition temperature (from 210 K up to 370 K). The performed ^{31}P NMR experiments demonstrate a great change in the relaxation times (T1 and T2) reflecting a significant slowing down of the dynamics for small pore systems in comparison with the bulk. Additionally, a detailed analysis of 1D spectra reveals pronounced dynamic heterogeneities, which we describe by a distribution of correlation times. The width of the latter decreases gradually while approaching the bulk limit. Furthermore, exploiting the large dynamic window of ^{31}P NMR, 2D exchange NMR is applied in order to establish whether the dynamic heterogeneities are of static or transient nature.

DF 6.3 Tue 10:15 EB 407

On the nature of the high-frequency relaxation in a molecular glass former: A joint study of glycerol by field cycling NMR, dielectric spectroscopy and light scattering — •Catalin Gainaru[1], Oliver Lips[2], Anna Troshagina[1], Robert Kahlau[1], Alexander Brodin[1], Franz Fujara[2], and Ernst A. Rössler[1] — [1]Experimentalphysik II, Universität Bayreuth, D-95444 Bayreuth — [2]Inst. f. Festkörperphysik, TU Darmstadt, Hochschulstraße 6, D-64289 Darmstadt

Recently we introduced a new approach to disentangle α-peak and excess wing (EW) contributions in the dielectric spectra of glass formers, assuming that the α-process obeys frequency-temperature superposition (FTS) in the full temperature range above the glass transition temperature T_g. Based on this scenario, a comparison between the orientational correlation functions of rank $l = 1$ (probed by dielectric spectroscopy – DS) and $l = 2$ (probed for the first time over a broad frequency range by field cycling NMR and light scattering – LS) is carried out. For the glass former glycerol DS, NMR and LS spectra are scaled according to FTS over 15 decades in frequency. Significant differences in the spectral shape of the susceptibilities of different ranks are recognized on both sides of the relaxation peak, while the time constants turn out to be the same. Regarding the systematic differences observed at high frequencies, they are explained by assuming that the fast dynamics (EW) proceeds via small angles. Below T_g, NMR and DS reflect the same dynamics down to cryogenic temperatures.

DF 6.4 Tue 10:30 EB 407

Dielectric polarization noise near the glass transition — •Sandra Jenewein, Andreas Fleischmann, Gernot Kasper, Andreas Reiser, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Dielectric polarization noise can reveal fundamental information on relaxation processes in glass forming liquids or glasses. We measured the voltage and current noise spectral density in the organic glass former tri-propylene glycol in the vicinity of the glass transition. A home built electrometer amplifier was used to measure the voltage fluctuations of a capacitor filled with the sample. Using a custom built current-to-voltage converter we measured the current fluctuations of the sample. From the noise spectra we determined the dynamic glass transition. Using the fluctuation-dissipation theorem a comparison to frequency domain dielectric spectroscopy will be given.

DF 6.5 Tue 10:45 EB 407

Glassy dynamics in the mono-, di- and trimer of glass-forming propylene glycol — •Melanie Köhler, Robert Wehn, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

We report broadband dielectric spectra on glass-forming propylene glycol and its di- and trimer. Aside of the α-relaxation, we focus on the dynamics at higher frequencies, which is believed to play an important role for the glass transition. While the monomer of propylene glycol has a well-developed excess wing, a characteristic spectral feature of glassy dynamics beyond the α-relaxation [1], the di-and trimers show a Johari-Goldstein β-relaxation [2]. Interestingly, as revealed by long-time aging experiments performed in our group [1], the excess wing in propylene glycol also can be described as signature of a β-relaxation. The data is analysed in the framework of different models, as the coupling model and the minimal model [3, 4]. In addition we treat the relation between the Cole-Cole peak, recently suggested within an extended version of mode coupling theory [5], and the spectral properties of the experimentally detected β-relaxation in these glass formers. Also first results in the region beyond GHz frequencies, where additional fast processes are expected, are provided. [1] K.L. Ngai *et al.*, J. Chem. Phys. **115**, 1405 (2001). [2] K. Grzybowska *et al.*, J. Chem. Phys. **125**, 044904 (2006). [3] K. L. Ngai, Comments Solid State Phys. 9, 127 (1979). [4] J. C. Dyre, N. B. Olsen, Phys. Rev. Lett. **91**, 155703 (2003). [5] W. Götze and M. Sperl, Phys. Rev. Lett. **92**, 105701 (2004).

DF 6.6 Tue 11:00 EB 407

The high frequency wing of the α-process as probed by depolarized light scattering — •Nikolaus Petzold, Alexander Brodin, and E. A. Rössler — Universität Bayreuth

We show that the "intermediate power law"recently observed in optical Kerr effect (OKE) measurements is equivalent with the excess wing from frequency-domain data long since known from dielectric spectroscopy (DS), and is an equally common feature in depolarised light scattering (DLS). From the OKE representation we find that the wing from OKE and DS data has a temperature independent exponent γ. Based on this behavior, we build a mastercurve from the literature OKE data and transform it into DLS representation. The mastercurve obtained that way fits nicely our DLS data. We are able to obtain a model independent crossover temperature for several liquids (benzophenone BZP, propylene carbonate (PC), glycerol (GY), propylene glycol (PG), ortho-terphenyl (OTP), decahydroisoquinolin (DHIQ)), at which temperature the onset of the wing first appears and which corresponds to a characteristic relaxation time of $\tau_x \approx 10$ns. In the high temperature range, where no wing is observable, the apparent width of the α-peak correlates with the relaxation strength of the fast dynamics and anticorrelates with fragility opposite to common wisdom.

DF 6.7 Tue 11:15 EB 407

Secondary relaxations in molecular glasses and polymers studied by 2D ^{2}H NMR — •Björn Micko[1], Dieter Bingemann[2], and Ernst Rössler[1] — [1]Experimentalphysik II, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Department of Chemistry, Williams College, Williamstown, MA 01267, USA

We present a two-dimensional (2D) ^{2}H exchange NMR study, attempting to clarify the geometry of the molecular motion involved in the secondary relaxation (β-process) of three glass formers: PMMA, polybutadiene and a mixture of decaline and chlorobenzene. Stimulated echo measurements of the orientational correlation function circumscribe the temperature range, in which the β-process is expected to dominate the spectra. In this range we will show by comparison with the spectra of o-terphenyl, which does not show a pronounced β-process, that the β-process is also clearly observable in the 2D NMR spectra below and somewhat above T_g, until upon further heating the structural relaxation (α-process) enters the time window of the experiment and gives rise to a convergence of the spectra. Whilst the time constants for the studied systems (obtained from dielectric spectrocopy) are very similar on the reduced temperature scale T_g/T, the dielectric relaxation strength differs for each system. In contrast the 2D NMR spectra turn out to be practically identical on the T_g/T scale - which implies strong similarities concerning time scale and underlying geometry of the motion. To get further insight on the reorientation angles involved, simple motional models will be compared against the

spectra.

DF 6.8 Tue 11:30 EB 407

Raman scattering in glasses and the boson peak — •Bernhard Schmid[1] and Walter Schirmacher[2] — [1]FB Physik, Univ. Mainz — [2]Phys.-Dept. TU München

Vibrational spectra of glasses as measured e.g. by inelastic neutron scattering exhibit at low frequencies ($\sim$ 1THz) an enhancement over Debye's ω^2 law ("boson peak"). Using a theory of light scattering from disordered materials developed recently [1,2], we show that the anomalous low-frequency Raman spectra observed in this frequency regime are *not* proportional to the density of states (as was widely believed) but are related to the disorder-induced self-energy function. The latter, in turn, can be related to the width of the Brillouin line in the same frequency regime.

[1] B. Schmid, Diploma thesis, TU München, 2007
[2] B. Schmid and W. Schirmacher, to be published

DF 6.9 Tue 11:45 EB 407

Fractional approaches in dielectric broadband spectroscopy — •Simon Candelaresi[1] and Rudolf Hilfer[1,2] — [1]ICP, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Institut für Physik, Universität Mainz, 55099 Mainz, Germany

A fractional approach is used to describe data from dielectric spectroscopy for several glassy materials. Using composite fractional time evolution propagators [1] a modified law for relaxation in glasses [2] is found that describes the experimental data for broadband dielectric spectroscopy [3]. Properties and solutions of some particular fractional differential equations (fDEQs) are investigated both for rational and irrational order. The laws of Debye, Kohlrausch, Cole-Cole, Cole-Davidson and Havriliak-Negami are compared with this new approach in frequency and time space.

[1] R. Hilfer; Time, Quantum and Information, L.Castell and O.Ischebeck (Eds.); Springer-Verlag Berlin 2003 p.235
[2] R. Hilfer Chemical Physics, **284**, 399 (2002)
[3] U. Schneider et al., Phys. Rev. E, **59**, 6924 (1999)

DF 6.10 Tue 12:00 EB 407

Collective atomic dynamics and relaxation processes in Al_2O_3 melt — •Sandro Jahn[1] and Paul A. Madden[2] — [1]GeoForschungsZentrum Potsdam, Telegrafenberg, 14473 Potsdam — [2]Chemistry Department, University of Edinburgh, Edinburgh EH9 3JJ, UK

The atomic dynamics of Al_2O_3 melt are studied by molecular dynamics simulation. The particle interactions are described by an advanced ionic interaction model that includes polarization effects and ionic shape deformations. The model has been shown to reproduce accurately the static structure factors $S(Q)$ from neutron and x-ray diffraction and the dynamic structure factor $S(Q,\omega)$ from inelastic x-ray scattering. Analysis of the partial dynamic structure factors show inelastic features in the spectra up to momentum transfers, Q, close to the principal peaks of partial static structure factors. The broadening of the Brillouin line widths is discussed in terms of a frequency dependent viscosity $\eta(\omega)$.

DF 7: Point defect spectroscopy and engeneering

Time: Tuesday 10:00–13:00 Location: EB 107

Invited Talk DF 7.1 Tue 10:00 EB 107

Modelling of Point Defects in Ferroelectric Materials — •Karsten Albe[1] and Paul Erhart[2] — [1]Institut f. Materialwissenschaft, Petersenstr. 23, TU Darmstadt — [2]Lawrence Livermore National Laboratory, Materials Science Division, USA

The properties of ferroelectric materials and their behavior in the presence of electric fields are intimately related to the presence of defects. Oxygen vacancies, for instance, play a key role in aging and fatigue impeding domain wall motion or by acting as local disturbances of the polarization Experimental investigations of point defect properties either provide averaged bulk data or very localized information and can therefore be ambiguous. Quantum mechanical calculations based on density functional theory (DFT), on the other hand, are capable of providing fundamental insights into the energetics of defects as well as their kinetic and electronic properties. In this contribution, two examples will be discussed. For the prototype material barium titanate (BT), DFT calculations are used for verifying established defect models which have been employed to explain the experimental observations (in particular, conductivity and diffusivity measurements). Moreover, the formation of di-vacancies is explored which is an important ingredient for understanding the deterioration of ferroelectric switchability. In the second part, the energy surface of unbound oxygen vacancies and oxygen vacancies complexed with Fe or Cu in lead titanate (PT) is studied. The results are utilized to interpret recent electron spin resonance experiments and discussed in the context of existing defect models.

Invited Talk DF 7.2 Tue 10:40 EB 107

Polarons in lithium niobate — •Ortwin Schirmer — FB Physik, Universität Osnabrück

$LiNbO_3$ is an extraordinary testing ground for various manifestations of polarons. The Li-substoichiometry of its congruently melting composition facilitates the formation of bound hole (O^-), bound single electron (Nb_{Li}^{4+}) and bound electron bi-polarons (Nb_{Li}^{4+} - Nb_{Nb}^{4+}). Also free electron polarons (Nb_{Nb}^{4+}) can be prepared. In all cases these polarons are small, i.e. the ranges of the carrier amplitude and related lattice distortions extend over about one bond length. On the basis of detailed experimental information on bound hole polarons in numerous oxide materials, methods established for color centers have recently been modified to interpret the details of the corresponding strong optical absorption bands. This approach is extended to electron polarons in $LiNbO_3$. It allows to understand the related phenomena, most of them known since a long time, from a common viewpoint. Among the treated features will be the interpretation of the peak energies and shapes of the optical absorption bands, the binding energies of bipolarons as well as their dissociation and recombination.

DF 7.3 Tue 11:20 EB 107

Local structure and symmetry of paramagnetic ions in microscopic and nanoscopic ferroelectric materials — •Emre Erdem[1], Kamil Kiraz[2], Mehmet Somer[2], and Rüdiger -A. Eichel[1] — [1]Eduard-Zintl-Institut, Technische Universität Darmstadt, D-64287 Darmstadt, Deutschland — [2]Koc University, Department of Chemistry, Rumelifeneri Yolu, Sariyer, 80910 Istanbul Turkey

In this work, multi-frequency (9.5 GHz up to 319 GHz) electron paramagnetic resonance (EPR) spectroscopy is used in order to study the role of aliovalent and isovalent functional centres and their impact on lattice vacancies in $PbTiO_3$ and $PbZr_xTi_{1-x}O_3$. The examination of nanocrystalline ferroelectrics with perovskite structure and the determination of their physical and chemical properties are one of the challenges of the solid state physics and material science due to their potential application in device technology. To determine the structural changes which occur in correlation with size effects and size driven phase transition in $PbTiO_3$, dielectric, Raman and multi-frequency EPR measurements were carried out on Cr, Fe, Gd and Cu doped micro- and nanopowders. Through the size-dependent multi-frequency EPR spectra the spin-Hamiltonian parameters were determined and correlated with structural investigations and dielectric measurements.

DF 7.4 Tue 11:40 EB 107

The effect of (Gd^{3+},Cu^{2+}) and (Gd^{3+},Fe^{3+}) Co-Doping on the Defect Chemistry of $PbTiO_3$ — •Michael Drahus[1], Rüdiger Eichel[1], Emre Erdem[1], Hans Kungl[2], and Michael Hoffman[2] — [1]Eduard-Zintl-Institut, Technische Universität Darmstadt, Germany — [2]Institut für Keramik im Maschinenbau, Universtität Karlsruhe

The effect of Co-doping $PbTiO_3$ with (Gd^{3+}, Cu^{2+}) and (Gd^{3+}, Fe^{3+}) on dopant cation association of oxygen vacancies is examined with multiply-frequency EPR. Also, the possibility of the Gd cation substuting on both the A and B site as a self compensating acceptor donor is explored. Acceptordonor codoping has shown encouraging results as a way to reduce the Polarization Fatigue in both thin film and bulk Ferroelectrics. Therefore an understanding of the defect chemistry initiated by these scenarios is important for determining the underlying

mechanism of polarization fatigue suppression

DF 7.5 Tue 12:00 EB 107

Influence of extrinsic defects on the recombination behavior of light-induced hole and electron polarons in $KNbO_3$ — •Bettina Schoke, Christoph Merschjann, Stefan Torbrügge, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

We study excitation and recombination processes of small hole and electron polarons in nominally pure and iron doped $KNbO_3$ samples by means of time–resolved excited–state–absorption (ESA) spectroscopy. The light–induced absorption $\alpha_{\mathrm{li}}(t)$ in the visible and infrared spectral–range is measured after optical excitation with intense ns laser pulses ($\lambda = 532\,\mathrm{nm}, \tau = 8\,\mathrm{ns}$). In nominally pure $KNbO_3$ we observe the formation and relaxation of free (Nb_{Nb}^{4+}) electron polarons and bound O^- hole polarons within a single decay of α_{li} after a two–photon process of excitation. Their mutual recombination via incoherent hopping transport is crucially accelerated by Iron doping which additionally causes a slow decay component in $KNbO_3$:Fe. The reduction of the polaron hopping transport length in Fe-doped samples can be attributed to the increased number densities of optically-generated O^- hole polarons by additional one-quantum excitations due to extrinsic defects.

Financial support by the Deutsche Forschungsgemeinschaft DFG (TFB 13-04, IM 37/2-2, GRK 695).

DF 7.6 Tue 12:20 EB 107

Solid-state NMR on defects in lead titanates — •Marko Bertmer[1], Rüdiger Eichel[2], and Hans Kungl[3] — [1]Experimentelle Physik 2, Leipzig, Deutschland — [2]Physikalische Chemie III, Darmstadt, Deutschland — [3]Institut für Keramik im Maschinenbau, Karlsruhe, Deutschland

Failure of ferroelectrics is not well understood. In our approach, we employ various solid-state NMR techniques to characterize and quantify chemical structures that arise from crystallographic defects. Especially, the existence and distributions of ^{1}H as water or other species is a primary goal in our research.

^{1}H spectra are known to be often of low resolution due to the strong homonuclear dipolar coupling. With sophisticated NMR techniques, e. g. echo methods and multiple quantum transitions, we want to get more insight into the defect structures. This enables both improvement in spectral resolution as well as to obtain information about the dynamics of present chemical structures such as water.

Additionally, all nuclei present in lead titanates are accessible by NMR with different degree of sensitivity. Especially, with self-built equipment we are able to increase the abundance of the ^{17}O nuclei and therefore allow for detection.

DF 7.7 Tue 12:40 EB 107

Gitterplatzbestimmung und Ausheilverhalten von Hf implantiertem CaF_2 — •Thomas Geruschke und Reiner Vianden — Helmholtz - Institut für Strahlen und Kernphysik, Nußallee 14-16, 53115 Bonn, Deutschland

Untersucht wurden Hafnium implantierte Kalziumfluorid Einkristalle der Firma Schott AG. Die Gitterschäden, die durch die Implantation entstanden sind, wurden mittels RBS (Rutherford back scattering) abgeschätzt. Der Gitterplatz der implantierten Hf Ionen wurde entlang der <110> Kristallachse durch Gitterführungsexperimente bestimmt. Diese Experimente zeigten, das sich direkt nach der Implantation die Hf Ionen hauptsächlich (ca. 90%) auf regulären Ca Gitterplätzen befinden. Ein Vergleich des RBS Winkelscans mit Monte Carlo Simulationen bestätigt dies.

Das Ausheilen der Implantationsschäden durch ein isochrones Temperprogramm wurde mittels der Methode der gestörten γ - γ Winkelkorrelation (PAC) untersucht. Es zeigte sich eine starke Quadrupolwechselwirkung mit einer Frequenz von ν_u=1200MHz (η=0.43) ab einer Ausheiltemperatur von 550°C. Der Ursprung dieser Wechselwirkung sind Punktdefekte in unmittelbarer Sondenumgebung. Ob es sich dabei um Fluorfehlstellen oder substitutionellen Sauerstoff auf Fluorplätzen handelt ist noch Gegenstand der Untersuchung.

DF 8: Glasses II (joint session DF/DY)

Time: Tuesday 14:30–16:15 Location: EB 407

DF 8.1 Tue 14:30 EB 407

Glassy Solution-Space Structure of Optimization Problems — Alexander Mann[1], Wolfgang Radenbach[2], and •Alexander Hartmann[3] — [1]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]University of Göttingen, Platz der Göttinger Sieben 5, 37073 Göttingen, Germany — [3]Institute for Physics, University of Oldenburg, 26111 Oldenburg, Germany

We study numerically the glassy solution-space cluster of random ensembles of two NP-hard optimization problems originating in computational complexity, the vertex-cover problem and the number partitioning problem. We use branch-and-bound type algorithms to obtain exact solutions of these problems for moderate system sizes. Using two methods, direct neighborhood-based clustering and hierarchical clustering, we investigate the structure of the solution space. The main result is that the correspondence between solution structure and the phase diagrams of the problems is not unique. Namely, for vertex cover we observe a drastic change of the solution space from large single clusters to multiple nested levels of clusters. In contrast, for the number-partitioning problem, the phase space looks always very simple, similar to a random distribution of the lowest-energy configurations. This holds in the "easy"/solvable phase as well as in the "hard"/unsolvable phase.

DF 8.2 Tue 14:45 EB 407

A Gaussian model for the energy landscape of supercooled liquids and its implications — •Andreas Heuer — Inst. f. Phys. Chemie, Corrensstr. 30, 48149 Münster

From the previous analysis [1,2] of the potential energy landscape of molten silica and of a binary Lennard-Jones system a simple picture has emerged for the properties of the potential energy landscape as well as the relation between the energy and the dynamics. Formulating these observations in a general framework one can make specific predictions about the behaviour of supercooled liquids. This involves the dependence of fragility to non-exponentiality, the invalidation of the Stokes-Einstein relation and the relation between thermodynamic and kinetic fragility.

[1] B. Doliwa, A. Heuer, Phys. Rev. Lett. 91, 235501 (2003). [2] A. Saksaengwijit, J. Reinisch, A. Heuer, Phys. Rev. Lett. 93, 235701 (2004).

DF 8.3 Tue 15:00 EB 407

Fluorescence lifetime fluctuations and molecular reorientation of single molecules as observables of the dynamics in supercooled poly(methyl acrylate) — Renaud Vallée[2], •Gerald Hinze[1], Taoufik Rohand[2], Noel Boens[2], Wim Dehaen[2], and Thomas T. Basché[1] — [1]Institute of Physical Chemistry, Johannes-Gutenberg University, Mainz, Germany — [2]Department of Chemistry , Katholieke Universiteit Leuven, 3001 Leuven, Belgium

The dynamics of supercooled poly(methyl acrylate) has been explored on a nanoscale by tracking single fluorescing molecules as local reporter. We could follow the molecular orientation and the fluctuating fluorescence lifetime of single dyes in time. To meet the requirements of high photostability and a very high quantum yield, custom-built BODIPY dyes have been used. Experiments were performed in bulk sample to prevent interface effects.

While the rotational dynamics of the dyes strongly depends on the interaction between matrix and the probe molecules, the fluorescence lifetime could alter solely by matrix fluctuations without structural dynamics of the dye. We have analyzed the fluctuations by means of correlation functions and discuss their relationship to the dynamics of the supercooled matrix.

DF 8.4 Tue 15:15 EB 407

Properties of the Incoherent Scattering Function as derived from a Continuous Time Random Walk Analysis — •Oliver Rubner and Andreas Heuer — Institut für Physikalische Chemie der Universität Münster

We have shown in previous work that it is possible to describe the dynamics of a binary mixture Lennard-Jones (BMLJ65) model system above the glass transition in terms of a continuous time random walk (CTRW). Here we focus on the connection to experimentally accessible quantities. Approximating the incoherent intermediate scattering function $F(q,t)$ as a stretched exponential function $\exp(-\left(\frac{t}{t_0}\right)^{\beta})$ we have been able to derive analytical expressions for the q-dependence of the two parameters $t_0(q)$ and $\beta(q)$. These expressions are well reproduced by simulations of the BMLJ65 system.

We analyse the behaviour of the resulting equations in different q-regimes and are able to interpret their physical content exhibiting close connections to existing work, e.g. on facilitated spin systems. Furthermore system size effects are discussed.

DF 8.5 Tue 15:30 EB 407

Finite size corrections in mean-field spin glasses — •Timo Aspelmeier[1], Alain Billoire[2], Enzo Marinari[3], and Michael A. Moore[4] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Service de physique théorique, CEA Saclay, 91191 Gif-sur-Yvette, France — [3]Dipartimento di Fisica, INFM and INFN, Sapienza Università di Roma, P. A. Moro 2, 00185 Roma, Italy — [4]School of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, UK

Finite size corrections in mean-field spin glasses are poorly understood theoretically because calculation of the loop expansion beyond Gaussian order is practically impossible. Here we present arguments and simulations to show that a system of finite size N is stabilized by a finite number of replica symmetry breaking steps K as opposed to the infinite replica symmetry breaking found in the thermodynamic limit. The number K is shown to be proportional to $N^{1/6}$. Using this correspondence between K and N we calculate the finite size dependences of internal energy, free energy, Edwards-Anderson order parameter and sample-to-sample fluctuations of the free energy.

DF 8.6 Tue 15:45 EB 407

The critical behavior of 3D Ising spin glass models: universality and scaling corrections — •Martin Hasenbusch[1], Andrea Pelissetto[2], and Ettore Vicari[3] — [1]Institut für theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig, Deutschland — [2]Dipartimento di Fisica dell'Universita di Roma I and I.N.F.N., I-00185 Roma, Italy — [3]Dipartimento di Fisica dell'Universita di Pisa and I.N.F.N., I-56127 Pisa, Italy

We perform high-statistics Monte Carlo simulations of three three-dimensional Ising spin glass models: the +-J Ising model for two values of the disorder parameter p, p=1/2 and p=0.7, and the bond-diluted +-J model for bond-occupation probability p_b = 0.45. A finite-size scaling analysis of the quartic cumulants at the critical point shows conclusively that these models belong to the same universality class and allows us to estimate the scaling-correction exponent omega related to the leading irrelevant operator, omega=1.0(1). We also determine the critical exponents nu and eta. Taking into account the scaling corrections, we obtain nu=2.53(8) and eta=-0.384(9).

DF 8.7 Tue 16:00 EB 407

The m-component spin glass on a Bethe lattice — •Axel Braun[1] and Timo Aspelmeier[2] — [1]Institut für theoretische Physik, Universität Göttingen — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Using an extension of the cavity method to m-component vector spins on a Bethe lattice, we have derived a self-consistent equation of cavity fields, with $m \to \infty$. We have improved these findings by calculating corrections for a finite number of spin components and used these self consistent field equations to investigate the distribution of cavity fields in the low temperature phase. We provide numerical evidence that the RS distribution is unstable for finite m slightly below the critical temperature, indicating a second transition to a RSB state.

DF 9: Poster

Time: Tuesday 15:00–18:00 Location: Poster G

DF 9.1 Tue 15:00 Poster G

Tuning the Li diffusivity of poor ionic conductors by mechanical treatment: High Li conductivity of nanocrystalline $LiTaO_3$ — •Viktor Epp, Martin Wilkening, Armin Feldhoff, and Paul Heitjans — Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Callinstr. 3-3a, 30167 Hannover

Lithium tantalate, $LiTaO_3$, with an average particle size in the μm range is known as a very poor Li ion conductor. It is shown that its Li conductivity can be drastically increased by ball-milling. The thus obtained nanostructured powder with an average particle size of about 20 nm shows a dc conductivity, σ_{dc}, of about $3 \cdot 10^{-6}$ S cm^{-1} at $T = 450$ K ($\sigma_{\mathrm{dc}}T = 1.4 \cdot 10^{-3}$ S cm^{-1} K) which is about five orders of magnitude larger than that of the corresponding microcrystalline powder at the same temperature. The activation energy E_{A} is reduced by about one third, i. e., it decreases from $E_{\mathrm{A}} = 0.90(1)$ eV to about $E_{\mathrm{A}} = 0.63(1)$ eV. Similar results were previously obtained for lithium niobate [1]. The effect of different milling times on the ionic conductivity is studied. Furthermore, the thermal stability of the nanocrystalline materials against grain growth has been checked by *in situ* impedance spectroscopy. Interestingly, the Li conductivity of a sample milled for 16 h does not change much even when the material is exposed to about 700 K for several hours. Moreover, the Li self-diffusion in the nanostructured as well as the coarse grained materials is elucidated by various solid-state ^{7}Li NMR techniques.

[1] P. Heitjans, M. Masoud, A. Feldhoff, M. Wilkening, *Faraday Discuss.* **134** (2007) 67.

DF 9.2 Tue 15:00 Poster G

Nanoporöse Festkörperfarbstoffhybride — •Jennifer Krause, Andrea Schuy, Theo Woike und Dominik Schaniel — 1.Physikalisches Institut , Universität zu Köln

Farbstofflaser können über einen großen Spektralbereich von ultraviolett bis ins nahes infrarot sowohl im CW-Modus als auch gepulst betrieben werden. Ein Festkörperfarbstoffmaterial hätte gegenüber den bisher in Farbstofflasern verwendeten Flüssigkeiten viele Vorteile. Eine Möglichkeit Festkörperfarbstoffmaterialien zu realisieren ist es die Farbstoffe in eine geeignete Matrix einzubetten. Diese Matrix muss eine hohe optische Qualität haben und in einem weiten Spektralbereich transparent sein. Ebenso soll sie eine hohe Zerstörschwelle gegenüber Laserstrahlung und eine große thermische- und photochemische- Stabilität aufweisen. Geeignete Matrizen die diese Ansprüche erfüllen sind Xerogele [1]. Wir haben Xerogele nach dem Sol-Gel Verfahren [2] hergestellt und sie mit Farbstoffen beladen. Mittels Lumineszenz Spektroskopie untersuchen wir, welchen Einfluss die Konzentration der Farbstoffe in den Gelen und die Porengröße der Gele auf die Lumineszenz Eigenschaften sowie die Lebensdauer der Laserfarbstoffe haben.

[1]E. Yariv, S. Schultheiss, T. Saraidarov, R. Reisfeld, Optical Materials vol.16, p.29 (2001)

[2] N. Hüsing, U. Schubert, Angewandte Chemie Int. Ed. vol. 37, p. 23 (1998)

DF 9.3 Tue 15:00 Poster G

Low-coherence microscopy versus projected fringe method for the study of surface topography of photo inkjet papers — •Kai Brune[1,2], Mirco Imlau[1], and A. Knittel[2] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]Felix Schoeller Service GmbH, Burg Gretesch, D-49086 Osnabrück

We have investigated the topography of photo inkjet paper surfaces in different production steps. The aim of our work was to optimize the paper quality and to find a method for quality assurance. The topography analysis of the surface was performed by low-coherence microscopy and projected fringe method. From the roughness and the surface analysis a correlation between the paper quality and the surface structure was found. The quality of the photo inkjet paper is defined by the quality of the paper surface and the printing characteristics. Both methods for surface analysis were compared and the advantages and disadvantages were discussed. Some basic information is presented on this poster. The studies were performed in cooperation with the Felix Schoeller Service GmbH in Osnabrück.

DF 9.4 Tue 15:00 Poster G

Interface properties of $PbTiO_3$ and PZT thin films on

Pt-terminated substrates — •Salah Habouti[1], Claus-Henning Solterbeck[1], Mohammed Es-Souni[1], Vladimir Zaporojtchenko[2], and Franz Faupel[2] — [1]Institute for Materials and Surface Technology, University of Applied Sciences Kiel — [2]Chair for Multicomponent Materials, Christian-Albrechts-Universtät zu Kiel

Electrical properties of $Pb(Zr_{0.52}Ti_{0.48})O_3$ (PZT) and $PbTiO_3$ thin films are influenced by processes at the interface with the substrate. These interfaces are investigated for sol-gel processed thin films on Pt-terminated substrates. XPS depth profiles from samples prepared at various temperatures and in situ XRD measurements at different temperatures reveal the stochiometry and transformation kinetics at the interfaces. An intermediate phase with Pt and Pb emerges at the beginning of the film formation, but it disappears completely when the crystallization is complete.

DF 9.5 Tue 15:00 Poster G

Transmission of light through subwavelength holes in thin metal films — •Mathieu Gentile[1,2], Felix Kalkum[1], Manfred Fiebig[2], and Karsten Buse[1] — [1]Physikalisches Institut, Wegelerstraße 8, 53115 Bonn, Germany — [2]Helmholtz-Institut für Strahlen- und Kernphysik, Nussallee 14 - 16, 53115 Bonn, Germany

It was discovered a decade ago that a hole array in a thin metal film with hole diameters much smaller than the wavelength, λ, exhibit a transmission efficiency, η, higher than 100% in the visible range. Here, η denotes the intensity of light transmitted through the hole in relation to the intensity incident onto the hole area. Unfortunately, a satisfactory understanding of the intensity enhancement has not been reached up to date. The present work is devoted to the experimental quantification of η for transmission through a single circular hole. In particular, phase-conjugation experiments, in which holograms are recorded in $LiNbO_3$ crystals by focusing light onto a small hole in a metal film, will benefit from this quantification. Thus, $LiNbO_3$ crystals are used as a substrate for a 200-nm-thick gold metal film illuminated by a 532-nm-frequency-doubled Nd:YAG laser. Using the knife-edge method a Gaussian profile with radius of 3.82 μm and total power of 81 mW is determined for the focused beam. A peak transmission efficiency of $(335 \pm 7)\%$ is observed for a 350-nm-diameter hole ($2r/\lambda$=0.66).

DF 9.6 Tue 15:00 Poster G

Formation of nanoporous alumina films in sulphosalicylic acid solution — •Piotr Hamolka[1], Igor Vrublevsky[1], Vitaly Sokol[1], and Liubou Hamolka[2] — [1]Department of Nano- and Microelectronics, BSUIR, Minsk, Republic of Belarus — [2]The Institute of General and Inorganic Chemistry of the NAS of Belarus, Minsk, Republic of Belarus

This work presents the results studying the volume expansion factor of porous alumina films, formed by through anodizing of an aluminum foil of 11.5 μm thickness in a 0.6M sulphosalicylic acid solution. The thickness of porous alumina films was measured by an optical microscopy. The volume expansion factor of nanoporous alumina films in the range of anodizing current densities of 1.0 * 60 mA cm^{-1} varied from 1.23 to 1.64. The obtained results demonstrated linear dependence for the current density logarithm versus the inverse volume expansion factor. The curve on this plot was found to be consisted of two subsequential rectilinear regions. We suggested that the change in the film oxide growth is the evidence of modification of the structure of Helmholtz layer in the sulphosalicylic acid electrolyte with increasing of anodizing current. The structure of oxide films obtained at different anodizing current densities was studied with thermogravimetric analysis.

DF 9.7 Tue 15:00 Poster G

Probing nanoscale ferroelectricity by photoemission - the $PbTiO_3$ / Nb-$SrTiO_3$ (100) system — •Eike F. Schwier[1], Laurent Despont[1], Céline Lichtensteiger[2], Claude Monney[1], Corsin Battaglia[1], Matthew Dawber[2], Gunnar Garnier[1], Jean-Marc Triscone[2], and Philipp Aebi[1] — [1]Institut de Physique, Université de Neuchâtel, CH-2000 Neuchâtel, Switzerland — [2]DPMC, Université de Genève, Switzerland

Ferroelectric thin films have become more and more important as possible substituents of ferromagnetic storage devices. To utilize these new materials within the lowered dimensionality of modern electronics, one has to investigate the limits of the films functionality. Two questions are especially important. Does a critical thickness for ferroelectricity exist? And what does the interaction of the electrodes with the film change inside the film?

We performed photoemission experiments on ultra thin $PbTiO_3$ films grown on Nb-$SrTiO_3$ (100) in order to probe the properties close to the surface and at the atomic scale. X-ray photoelectron diffraction maps are used to probe the intra-cell polar atomic distortion and tetragonality associated with ferroelectricity at the surface. Thickness and mean detection depth dependencies in X-ray photoelectron spectroscopy data lead to a semi-classical model which might be able to describe the electrostatic potential course across the system. To estimate the influence of sample charging versus the charge displacement created by the ferroelectricity, a time and intensity dependent shift in the photoelectron kinetic energy is exploited.

DF 9.8 Tue 15:00 Poster G

Soft, flexible and conformable ferroelectret touchpad — •Gerda Buchberger, Reinhard Schwödiauer, and Siegfried Bauer — Soft Matter Physics, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Flexible electronics is a driving impetus in plastic electronics. Besides displays, electronic components are required for the communication between the human users and the device, examples include touchpads or touchscreens. To be used in plastic electronics, such elements should be prepared as easy as possible, thereby complex array constructions of sensors are outruled. Here we describe a very simple, soft, flexible and conformable touchpad based on cellular ferroelectrets with a strong longitudinal piezoelectric effect. Thereby the device is insensitive to bending piezoelectricity and only activated by the touch of a user. Instead of array sensors, a large area sensor element is described with electronic components at the periphery. In order to determine the minimum number of electronic elements at the periphery, topological and symmetry arguments are employed. In addition the symmetry breaking of ferroelectrets along the thickness direction of the foil may be used to advantage. We describe a simple single touch input/output device, and present first investigations of the characteristics of the element. Work partially supported by the FWF.

DF 9.9 Tue 15:00 Poster G

Charge transport in composite-materials containing carbon nano-tubes and carbon nano-fibers — •Michael Konter[1], Pablo Carballeira[2], Frank Haupert[2], Bernd Wetzel[2], Alois K. Schlarb[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We have investigated the electric transport properties of composite materials using temperature dependent dielectric spectroscopy (200 Hz - 2 GHz, 70 K - 290 K). The samples consist of epoxy-resin containing up to 2 vol. % carbon nano-tubes and carbon nano-fibers, respectively. The dispersion was achieved with a torus mill and / or a three roll calender device. We observe percolation as well as an associated polarization process. Its characteristic frequency and its dielectric strength are correlated with the dc-conductivity. This behaviour is discussed in terms of the micro-structure.

DF 9.10 Tue 15:00 Poster G

Investigation of the uniaxial relaxor calcium barium niobate by k-space spectroscopy and pyroelectric methods: a comparison to strontium barium niobate. — •Urs Heine[1], Uwe Völker[1], Klaus Betzler[1], Manfred Burianek[2], and Manfred Mühlberg[2] — [1]University of Osnabrück, Department of Physics, Barbarastr. 7, 49076 Osnabrück — [2]University of Cologne, Institute of Crystallography, Zülpicher Str. 49b, 50674 Cologne

The ferroic relaxor strontium barium niobate (SBN) has been considered as a promising material for optical applications, but the low phase transition temperature region prevents reliable utilization of its ferroelectric characteristics. Here, we present comparative investigations of the unfilled tungsten bronze calcium barium niobate (CBN) using k-space spectroscopy and pyroelectric measurements. Contrary to SBN, CBN shows a limited stability region in the range of about 20 and 40 mole fraction calcium. Congruently melting CBN (28.1 mole fraction calcium [1]) shows a relaxor phase transition analog to that in SBN at approximately 540 K, 200 K higher than that of SBN61. By applying external electric fields to CBN, we find similar behaviour as for SBN [2], even though the anisotropy in the distribution of the domainsizes arises at higher fields. Thus, we conclude that CBN - like SBN - exhibits a domain size dependent ferroelectric characteristic, too.

[1] M. Burianek, B. Joschko, I. Kerkamm, T. Schoenbeck, D. Klimm, M. Muehlberg: J. Crystal Growth 229, 413-417 (2007)

[2] U. Voelker, U. Heine, C. Gödecker, K. Betzler: Journal of Applied Physics: in print (2007)

DF 9.11 Tue 15:00 Poster G

Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscope — •Philipp Schreier[1], Lothar Kador[1], Deliani Lovera[2], and Volker Altstädt[2] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth — [2]University of Bayreuth, Department of Polymer Engineering, 95440 Bayreuth

We present a custom-built set-up capable of performing three-dimensional confocal Raman and fluorescence lifetime imaging (FLIM) microscopy. 3-d Raman measurements were performed on spider silk fibers and electro-spun electret fibers which were prepared from miscible and non-miscible polymer mixtures. In both cases of the electret materials, the compositions of the fibers were homogeneous on the micrometer scale. For the FLIM experiments the cw laser is modulated with an acousto-optic modulator in the MHz regime, and the phase shift of the fluorescence light with respect to the excitation is measured. In this way, fluorescence lifetimes in the nanosecond range can be obtained. First data of, e. g., paper samples stained with different fluorescent dyes are presented.

DF 9.12 Tue 15:00 Poster G

Topographic investigations of LiB_3O_5-crystal surface degradations generated at reduced and normal pressure — Stefan Möller, •Änne Andresen, and Mirco Imlau — Department of Physics, University of Osnabrück, D-49069 Osnabrück

We have investigated the degradation of LiB_3O_5-crystal surfaces during long-term irradiation with intense laser light of $\lambda = 355\,\mathrm{nm}$, $\lambda = 532\,\mathrm{nm}$, or $\lambda = 1064\,\mathrm{nm}$ wavelength, and different repetition rates up to 100 kHz as well as cw-light. The topographic analysis of the surfaces were performed with low-coherence and atomic-force microscopy. At reduced pressure a catastrophic degradation of the surface was already observed upon irradiation with green light, whereas at normal pressure UV-radiation was necessary for the generation of surface degradation. The surface degradation emerge faster upon increase of the light intensity. A model for the generation of the observed surface degradations related to thermal damage will be presented. The general applicability of low-coherence microscopy as a method to analyze light-induced degradations of LiB_3O_5-crystal surfaces is considered. Financial support by the DFG (TFB 13, project A5/13-04).

DF 9.13 Tue 15:00 Poster G

Influence of Mg-doping on the lifetime of optically generated small polarons in $LiNbO_3$ — •Daniela Conradi[1], Bettina Schoke[1], Christoph Merschjann[1], Mirco Imlau[1], Gabor Corradi[2], and Katalin Polgár[2] — [1]Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany — [2]Hungarian Academy of Sciences, Budapest, Hungary

Excitation and recombination of optically generated small electron and hole polarons in Mg-doped $LiNbO_3$ is investigated by means of time-resolved excited-state-absorption (ESA) spectroscopy. Transient light-induced absportion changes $\alpha_{\mathrm{li}}(t)$ are observed in the visible and near infrared spectral range upon excitation with intense green laser pulses ($\lambda = 532\,\mathrm{nm}, \tau = 8\,\mathrm{ns}, I_\mathrm{p} \leq 1400\,\mathrm{GW/m^2}$). The results indicate the generation of bound small O^- hole polarons and bound small Nb_{Li}^{4+} electron polarons in $LiNbO_3$:Mg with doping concentrations below the optical-damage-resistance threshold. In contrast, for concentrations above this threshold the light-induced absorption is caused by hole polarons and free small Nb_{Nb}^{4+} electron polarons. In either case the characteristics of $\alpha_{\mathrm{li}}(t)$ in the blue-green spectral range point to the presence of further extrinsic impurities — most likely $Fe^{2+/3+}$.

We present a model concerning all these types of polarons for $LiNbO_3$ doped with Mg below and above the optical-damage-resistance threshold. The influence of additional extrinsic impurities on the excitation and recombination of the small polarons is discussed.

Supported by the Deutsche Forschungsgemeinschaft (Projects IM 37/2-2 and TFB 13-04).

DF 9.14 Tue 15:00 Poster G

Amplitude-Frequency-Characteristics 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 poster presents amplitude-frequency-characteristics (AFC) observed at different types of thin film samples (Metal/Ferroelectric/Metal and Metal/Ferroelectric/Semiconductor). The differences among them are pointed out and a comparison is made with respect to the typical response of a ferroelectric bulk material.

The results show, how hysteresis and its transient alterations due to fatigue manifest in a shift of resonance frequency. This behaviour can be simulated numerically, and thus explain the observed deviations of the AFC from a linear response.

DF 9.15 Tue 15:00 Poster G

Interfacial ion conduction in nanostructured solid electrolytes measured by Electrostatic force microscopy — •Ahmet Taskiran[1], Andre Schirmeisen[1], Bernhard Roling[2], and Bracht Hartmut[3] — [1]Physikalisches Institut,Wilhelm-Klemm-Str.10,48149 Münster,Germany — [2]Institut für Phys.Chemie,Hans-Meerwein-Str.,35032 Marburg,Germany — [3]Institut für Materialphysik, Wilhelm-Klemm-Str.10,48149 Münster,Germany

Solid ion conductors are applied in super-capacitors, high energy storage batteries and chemical sensors. Recent work has shown an enhancement of the overall conductivity by interfaces between different materials. Since the macros. measurements yield an average value over a large regime, an investigation on nanoscopic scale is needed to understand the ion dynamic. We use electrostatic force microscopy (EFM) operating in the noncontact mode, which use a sharp tip with an apex radius of 10 nm as measuring sensor. Therefore, the investigations of ion transport occur in nanoscopic volume. The investigation of temperature dependent ion conductivity was monitored in the range from 100-675 K, yielding the activation energies of the ion hopping process [1]. We measured the activation energies of nanocrystallites as well as the glass matrix in a partially crystallized LiAlSiO sample, which are in good agreement with macroscopic results [2] and identified an additional activation energy which can be attributed to the ions at the interface between both phases [3].[1]Schirmeisen et al.,Appl. Phys. Lett.85(2004)2053 [2]Roling et al.,Phys.Chem.Chem.Phys.7(2005)1472 [3]Schirmeisen et al.,Phys.Rev.Lett.98(2007)225901

DF 9.16 Tue 15:00 Poster G

First-principles investigation of thin $ATiO_3$ films with stacking faults — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The ferroelectric polarization is a fundamental quantity which is used for the realization of nanoelectronic devices applicable in information technology. Experimental studies have shown that defects and stacking faults play an important role in ferroelectric materials. Employing density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as realized in the FLEUR code (www.flapw.de), we study the polarization of thin films of the perovskite $ATiO_3$ compounds $PbTiO_3$ and $BaTiO_3$. Both AO-terminated and TiO_2-terminated surfaces with the polarization in the film plane or perpendicular to the surface are considered. We present studies on the applicability of different exchange-correlation potentials and first results on the influence of stacking faults at the surfaces on the ferroelectric polarization in these compounds.

DF 9.17 Tue 15:00 Poster G

Antiferroelectric / ferroelectric $PbZrO_3$ / $Pb(Zr_{0.8}Ti_{0.2})O_3$ multilayers: properties and effects — •Ksenia Boldyreva[1], Lucian Pintilie[1,2], Andriy Lotnyk[1], Nikolai Zakharov[1], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany — [2]NIMP, P.O. Box MG-7, 077125 Bucharest-Magurele, Romania

Epitaxial antiferroelectric / ferroelectric $PbZrO_3$ / $PbZr_{0.8}Ti_{0.2}O_3$ (PZO/PZT) multilayers (MLs) were grown by pulsed laser deposition on $SrTiO_3$(100) substrates, covered with a $SrRuO_3$ (100) bottom electrode and a thin tetragonal $PbZr_{0.2}Ti_{0.8}O_3$ buffer layer. Hysteresis, switching current-voltage and capacitance-voltage curves of the MLs with an individual layer thickness above 10 nm show a mixed AFE-FE behavior, whereas below 10 nm the MLs show only FE behavior. Obviously the $PbZrO_3$ layers thinner than 10 nm underwent a transition into the ferroelectric state with a corresponding symmetry change from orthorhombic to rhombohedral. An X-ray diffraction ϑ-2ϑ scan and Reciprocal Space Mapping showed a corresponding orthorhombic-to-rhombohedral transition of the $PbZrO_3$ layers [1]. High-resolution TEM images were taken in order to investigate the microstructure of the PZO/PZT multilayers. The observations are discussed in terms of a strain effect.

[1] K. Boldyreva, L. Pintilie, A. Lotnyk, I. B. Misirlioglu, M. Alexe, and D. Hesse, Appl. Phys. Lett. **91**, 122915 (2007)

DF 9.18 Tue 15:00 Poster G

Effects of MoO_3 and WO_3 on phase separation of a soda-lime-silica glass — •Rainer Kranold[1] and Armin Hoell[2] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Hahn-Meitner-Institut Berlin, D-14109 Berlin, Germany

The base glass, $13Na_2O$-$11CaO$-$76SiO_2$, undergoes subliquidus phase separation. Below the binodal temperature, T_b, the glass separates into two amorphous phases, silica enriched droplets and a silica-poor matrix. The phase separation process is governed by two competitive parameters, the thermodynamic driving force, $\Delta\mu$, and the interface tension, σ. Here, the effects of small MoO_3 and WO_3 additions to the base glass on the parameters $\Delta\mu$ and σ are investigated. By determination of the wetting angle of a drop of the liquid glass melt on the flat surface of pure silica glass it was found that additions of MoO_3 or WO_3 to the base glass increase the value of σ. The growth process of the droplets at 600 °C in glasses with and without MoO_3 or WO_3 was studied by small-angle X-ray scattering (SAXS). All of the glass samples were in the early stage of diffusion controlled coarsening. However, while in the pure glass the volume fraction, w, of the droplets continuously approaches its reported equilibrium value, w_e, the w values of the doped glasses exceed considerably the value of w_e. These findings can be explained by the assumption that the additives MoO_3 and WO_3 give rise to an increase of $\Delta\mu$ resulting in a shift of the miscibility gap to higher temperatures. By means of in situ high-temperature SAXS experiments, it was proved that T_b of the doped glasses is really increased in relation to that of the base glass.

DF 9.19 Tue 15:00 Poster G

Polarisationseffekte in dielektrischen Substraten — •bernhard faber — Institut für theoretische Physik 2, Uni. Erlangen, Deutschland

Durch Metallcluster ausgelöste Polarisationseffekte in dielektrischen Substraten werden behandelt. Untersucht werden Na_N-Cluster ($N < 10$) auf Cu(111) bzw. auf Ar-Schichten, die wiederum auf Cu(111) abgelegt werden.

Die Beschreibung des Clusters und der Oberfläche erfolgt in einem hierarchischen TD-DFT-MD-Modell. Die Valenzelektronen der Na-Atome werden mittels TD-LDA behandelt. Die Ankopplung der Na^+-Ionen und des Ar-Substrats erfolgt mit Hilfe lokaler Pseudopotentiale. Die Polarisationswechselwirkung des Cu-Substrats mit dem Na- und Ar-Adsorbat wird durch Bildladungen vermittelt.

Wir berechnen Schnitte durch die Born-Oppenheimer-Flächen. Im Fall zwischenliegender Ar-Layer werden Druckeffekte auf das Argon beobachtet. Ohne Pufferung ergibt sich ein Transfer von Elektronendichte ins Metall, und damit eine starke Polarisierung des Clusters.

DF 10: Glasses III (joint session DF/DY)

Time: Wednesday 14:30–16:15 Location: EB 407

DF 10.1 Wed 14:30 EB 407

Impedance- and IR-spectroscopy on sputtered borate glasses — •Gerd-Hendrik Greiwe and Guido Schmitz — Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster

Ion-conducting oxide glasses are considered as components of thin film batteries. In our study, glass films of the compositions $x\ Li_2O \cdot (1-x)\ B_2O_3$ with $x = 0.15$, 0.20, 0.25, 0.30, and 0.35 are prepared by ion beam sputtering in a thickness range between 100 and 1000 nm. TEM cross section investigations show a homogeneous, amorphous structure of the films, while the correspondence of their chemical composition with the glass targets is proved by EELS analysis. The specific dc-conductivity of the glass films is determined by temperature-dependent impedance spectroscopy and found to be up to three orders of magnitude higher compared to the conductiviy of the corresponding bulk glasses prepared from the melt. This conductivity increase is explained by a modification of the network structure of the thin glass films. The concentration of the Non-Bridging Oxygen atoms of the network is assumed to be increased by the sputter process. This increase is expected to be the main reason for the observed conductivity enhancement. IR-spectroscopy is used to determine the content of the Non-Bridging Oxyges atoms of the network, to correlate structural and electrical properties of the thin film glasses.

DF 10.2 Wed 14:45 EB 407

Decoupling of Atomic Diffusion in Glass-Forming Mixtures — •Thomas Voigtmann and Jürgen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

The diffusion in dense binary soft-sphere mixtures with disparate sizes is studied. While the system approaches a glass transition, only the transport of large particles ceases, while small particles are still able to diffuse through the almost frozen background formed by the large ones, leading to an order-of-magnitude decoupling in the respective transport coefficients. This mechanism qualitatively describes the phenomenology of ion-conducting melts such as sodium silicate mixtures. Upon further increasing the density, the small-particle mean-squared displacement shows an increasing regime of anomalous power-law-like diffusion, which is interpreted as the precursor of a second localization transition following the glass transition in this system.

DF 10.3 Wed 15:00 EB 407

In-situ study of dynamics in hydrous silicate melts with quasielastic neutron scattering — •fan yang[1], andreas meyer[2], tobias unruh[3], and josef kaplonski[1] — [1]Physik-Department E13, TU München, 85748 Garching, Germany — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51147 Köln, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TU München, 85748 Garching, Germany

Dissolved water in silicate melts and glasses is of great interest in geoscience as well as in technical applications. We investigate water dynamics in silicate melts and the correlation between macroscopic properties like viscosity and the microscopic structure. With the intrinsic q resolution of quasielastic neutron scattering diffusion can be studied in great detail. Diffusion of water in sodium trisilicate melt was studied in-situ at different temperatures under a pressure of 200 MPa. The temperature dependence of the H diffusion coefficient obeys an Arrhenius law with an activation energy of about 0.36 eV.

DF 10.4 Wed 15:15 EB 407

Conductivity of Alkali Glasses in Quantum Statistics — •Joachim Sohns and Michael Schulz — University of Ulm

Our aim is to find an analytically solvable model of the conductivity of mixed alkali glasses. Our starting point is the schroedinger equation of the multy particle wave function of the system. As a consequence of the structural and dynamical disorder the system is irreversible in time. The dynamics of the system is given by the matrix greens functions of the keldysh technique. The linear response of the system to an external electrical field may be calculated within the kubo formalism. In addition to the usual paramagnetic and diamagnetic current we find an other contribution to the current which is caused by the finite life times of the states. The dependence of the conductivity on the concentration of alkali ions, on the temperature and on the frequency of the external electrical field are calculated. The mixed alkali effect is reproduced by our model.

DF 10.5 Wed 15:30 EB 407

Barium diffusion in mixed cation glasses — •Michael Grofmeier, Frank Natrup, and Hartmut Bracht — Institute of Materials Physics, University of Münster, Germany

Diffusion of barium in mixed cation glasses of the composition xNa_2O*(3*x)BaO*4SiO_2 with x = 0.0, 0.1, 0.3 and 1.0 and 0.4K_2O*2.6BaO*4SiO_2 was investigated by means of the radiotracer diffusion technique below the respective glass transition temperatures. In accord with our previous results of calcium diffusion in soda-lime silicate glasses, the mobility of alkaline-earth ions increases with the alkali content in all analyzed glass systems with no decrease in the diffusion activation enthalpy, but a raise in the pre-exponential factor. A distinct dependency of the activation enthalpy of alkaline-earth ions on the type and content of the alkali ions in the glass is observed.

The results provide evidence for elastic and electrostatic contributions to cation diffusion in glasses and support the formation of dissimilar cation pairs, that were derived from nuclear magnetic resonance investigations of soda-lime silicate glasses and glasses containing sodium and barium. Finally, a striking correlation between the pre-exponential factor of alkaline-earth ion diffusion in soda-lime and potassium barium glasses is found whose origin remains unsolved.

DF 10.6 Wed 15:45 EB 407

Ion Dynamics in Room Temperature Ionic Liquids — Monika Mutke, •Radha Dilip Banhatti, and Klaus Funke — Institut für Physikalische Chemie und SFB 458, Universität Münster, Corrensstr. 30, D-48149 Münster

Room temperature ionic liquids (RTIL) are molten salts consisting of a bulky organic cation such as 1-butyl-3-methyl-imidazolium (BMIM) and anions such as BF_4^- and PF_6^-. Above T_G, RTILs exhibit non-Arrhenius type DC conductivities and are classified as of intermediate fragility. Earlier, the broadband conductivity spectra of a fragile ionic melt [1] and of a polymer electrolyte [2] were modelled providing a link between the short-time and the long-time dynamics of the ions, via the dispersive features of the spectra. We could thus obtain the activation energy of the elementary displacive step, E^*. In this contribution, we present and analyse the conductivity spectra of $BMIMBF_4$ from 1 mHz up to about 6 GHz in the temperature range 193 K - 353 K. We show that $BMIMBF_4$ exhibits spectral features similar to those of the polymer electrolyte, indicating the importance of structure mediated ion-ion interactions. Moreover, both for $BMIMPF_6$ and $BMIMBF_4$, E^* is found to be about 0.18 eV, which is similar to the conformational reorientation energy of the cation [3].

[1] P. Singh, R.D. Banhatti and K. Funke, Phys. Chem. Glasses **46**, 241 (2005).
[2] S.J. Pas, R.D. Banhatti and K. Funke, Solid State Ionics **177**, 3135 (2006).
[3] A. Rivera and E. Rössler, Phys. Rev. B **73**, 212201 (2006).

DF 10.7 Wed 16:00 EB 407

Crystal precursor nucleation: A connection between crystallization and vitrification. — •Hans Joachim Schöpe[1], Gary Bryant[2], and William van Megen[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland — [2]Department of Applied Physics, Royal Melbourne Institute of Technology, GPO Box 2476V, Melbourne 3001, Australia

A complete understanding of the solidification process (crystallization, vitrification) is one of the long-standing problems in condensed matter physics. The use of colloidal model systems provides an ideal controlled experimental system to reduce this lack of knowledge. We investigated the solidification scenario in suspensions of colloidal hard spheres for three polydispersities between 4.8% and 5.8%, from near freezing to near the glass transition. We identify four stages in the crystallization process: (i) an induction stage where large numbers of precursor structures are observed; (ii) a conversion stage as precursors are converted to close packed structures; (iii) a second nucleation stage; and (iv) a ripening stage. Near the glass transition the crystallization process is entirely frustrated, and the sample is locked into a compressed crystal precursor structure. Interestingly neither polydispersity nor volume fraction significantly influence the precursor stage, suggesting that the crystal precursors are present in all solidifying samples. We speculate that these precursors are related to the dynamical heterogeneities observed in a number of dynamical studies linking the two processes of crystallization and vitrification. JCP 127, 084505 (2007)

DF 11: Dielectric and ferroelectric thin films and nanostructures I

Time: Wednesday 14:00–17:00 Location: EB 107

DF 11.1 Wed 14:00 EB 107

The impact of strain on the properties of ferroelectric bilayers: A LGD approach — •Ludwig Geske, I.B. Misirlioglu, Ionela Vrejoiu, Marin Alexe, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120

Interfaces and defects may significantly alter the properties of ferroelectric thin films. Epitaxial bilayers consisting of $PbZr_{0.2}Ti_{0.8}O_3$ (*PZT20/80*) and $PbZr_{0.4}Ti_{0.6}O_3$ (*PZT40/60*) were grown by pulsed laser deposition with the scope to create defects in a controlled manner in order to investigate their influence. The films were deposited on vicinal $SrTiO_3$ (001) substrates using a perovskite $SrRuO_3$ bottom electrode which grows pseudomorphically to the subtrate. A large impact of the layer sequence on the defect generation and the formation of an a/c domain structure can be observed. These structural changes lead to a strong shifting of the remanent polarisation and the dielectric constant. In the attempt to understand this behaviour, the Landau-Ginzburg-Devonshire (LGD) theory is used, which is a versatile tool to describe the behaviour of ferroelectric materials. A short introduction into the LGD theory modified for the treatment of ferroelectric thin films will be given together with the results for single layered *PZT20/80* and *PZT40/60* films. Subsequently the influence of the electrostatic coupling at the interface between the *PZT* layers will be demonstrated. Finally the theory will be applied to the specific case of the *PZT* bilayers on $SrTiO_3$ to find an explanation for the behaviour of the ferroelectric properties by adapting the possible relaxation states and coupling terms.

DF 11.2 Wed 14:20 EB 107

Ferroelectricity in antiferroelectric epitaxial $PbZrO_3$ films with different orientations — •Ksenia Boldyreva[1], Lucian Pintilie[1,2], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany — [2]NIMP, P.O. Box MG-7, 077125 Bucharest-Magurele, Romania

$PbZrO_3$ (PZO) is a well known antiferroelectric (AFE) material with orthorhombic crystal structure. Due to antiparallel lead-ion shifts the remnant polarization is nominally zero. With a sufficiently large applied electric field, PZO undergoes a field-driven phase transition into a ferroelectric (FE), rhombohedral phase. However, the existence of a FE polarization along the c-axis of PZO (without applied field) was predicted by Jona *et al.* with an estimated value of 25 $\mu C/cm^2$ [1]. We have investigated the temperature dependence of hysteresis and capacitance in PLD-grown epitaxial PZO films with two different orientations in the 4.2-400K temperature range. It was observed that $(120)_o$-oriented films (index o-orthorhombic) show a mixed AFE and FE behaviour on the entire temperature range, the FE behaviour being more stable at low temperatures. In contrast, the $(001)_o$-oriented films show a FE hysteresis only at temperatures up to 60 K. Above 60 K the hysteresis splits into two loops, typical for antiferroelectrics. The results indicate the coexistence of FE and AFE properties in PZO films, particularly at low temperature.

[1] F. Jona, G. Shirane, F. Mazzi, and R. Pepinsky, Phys. Rev. **105**, 849 (1957)

DF 11.3 Wed 14:40 EB 107

Static and Dynamic Properties of Ferroelectric Nanostructures and Multiferroic Bulk Systems: A Multiscale Approach — •Thomas Michael[1], Julia Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-University, D-06099 Halle, Germany — [2]University of Sofia, Department of Physics, Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria

Ferroelectric nanostructures and multiferroic bulk systems are studied in a multiscale approach. The excitation energy and the associated damping of ferroelectric modes as well as the polarization and the hysteresis are presented as a function of the temperature, the defect concentration, size and shape of the nanomaterials. The softening of the mode is strongly influenced by the kind of doping ions, the surface configuration and the defect composition. The analysis is based on a modified Ising model in a transverse field. A Green's function technique in real space provides the static and dynamic properties, which differ significantly from the bulk behavior. Additionally a mesoscopic approach is carried out similar to the Landau-Lifshitz equation with Gilbert damping for ferromagnets. The temperature dependence of the damping paramters is discussed. The analysis is extended to multiferroic bulk systems, where the magnetic moments interact via the Heisenberg model and the multiferroic coupling term differs for hexagonal and orthorhombic materials. We present the dielectric function

and the dynamic properties of the coupled model. Both, the Green's function technique and the mesoscopic Landau-Lifshitz equation are applicable here. Theoretical results are compared with experiments.

DF 11.4 Wed 15:00 EB 107

Ferroelectric lithography on doped $LiNbO_3$ single crystals — •Alexander Haussmann 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 nanostructure assembling. Recent work has reported on the photochemical adsorption of noble-metal nanoparticles to such surfaces serving as pin-points for attaching desired organic molecules [1].

Here, we report on the formation of domain structures of μm-sizes in 5 mol% Mg-doped congruent $LiNbO_3$ single crystals by (a) UV-induced poling using a HeCd laser beam ($\lambda = 325$ nm) focused through liquid electrodes, as well as (b) the application of high voltage between a contact mode AFM tip and a back electrode. Subsequently, the deposition of wire-like metal structures at the domain wall positions was stimulated by illuminating the sample dipped into aqueous solutions of $AgNO_3$ or $Pt(NO_3)_2$ by super bad-gap illumination ($\lambda < 310$ nm) using a Hg spectral lamp. Structural properties of the resulting nano- and mesowires were examined using non-contact AFM and Kelvin probe force microscopy [2]. Electrical conductivity of 300 μm long Pt wires between macroscopic electrodes could be demonstrated by performing I-V-scans.

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

[2] U. Zerweck, Ch. Loppacher et al., Phys. Rev. B **71**, 125424 (2005)

DF 11.5 Wed 15:20 EB 107

Electron emission from ferroelectric thin films induced by polarization switching — •Oliver Mieth[1], Hannes Klumbies[1], Günter Milde[2], Gerald Gerlach[2], and Lukas Eng[1] — [1]Institut für Angewandte Physik, Technische Universität Dresden — [2]Institut für Festkörperelektronik, Technische Universität Dresden

Ferroic materials are promising candidates for high-efficient electron emission in various applications. However, most work in this research field so far did focus on electron emission from bulk ferroelectric materials.

Here we present studies on electron emission under ultra-high vacuum conditions (base pressure $< 10^{-9}$ mbar) using PZT and other thin ferroelectric films as the emitter source that measure some hundred nanometer in thickness. Electron emission is collected through 10 - 20 μm-sized apertures lithographically manufactured into the top electrode. We show that current densities of up to 10^{-11} A/cm^2 are measurable by simply switching the thin film in the 10 Volt regime. The count rates measured as a function of applied switching voltage showed an almost linear behavior, in contrast to bulk PMN-PT single crystals which exhibited an exponential relationship. For correlating these results to known ferroelectric properties, e.g., coercive field and local imprint effects, local hysteresis loops were recorded simultaneously using Piezoresponse Force Microscopy. We are able to demonstrate that polarization switching induces the onset of electron emission. These experimental findings were consistently interpreted using Finite Element Method (FEM) modeling of the investigated structure.

DF 11.6 Wed 15:40 EB 107

Field effect transistor of graphitized polyimide with P(VDF-TrFE) as gate insulator — •I. Lazareva[1], Y. Koval[1], P. Müller[1], I. Paloumpa[2], K. Müller[2], and D. Schmeisser[2] — [1]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany — [2]Lehrstuhl Angewandte Physik/Sensorik, Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus, Germany

Surfaces of polyimide films were graphitized by low-energy ion irradiation. The conductivity was between 10^{-5} to 200 S/cm [1]. We prepared field effect transistors using this material. Ferroelectric P(VDF-TrFE) was used as gate insulator. The thickness of P(VDF-TrFE) varied from 120 nm to 1200 nm. Properties of P(VDF-TrFE) were investigated by current-voltage measurements of metal/ P(VDF-TrFE)/metal capacitors. We have found that at room temperature, the coercive field of P(VDF-TrFE) does not depend on the film thickness. At lower temperatures the coercive field increases proportionally to the reciprocal temperature. Remnant polarization is 9.5 μC/cm^2. It slightly rises with decreasing temperature. Our recent results of field effect mobility, carrier concentration and threshold voltage are presented.

[1] I. Lazareva, Y. Koval, M. Alam, S. Strömsdörfer, P. Müller, Appl. Phys. Lett. 90, 262108 (2007)

DF 11.7 Wed 16:00 EB 107

Investigations on ferroelectric properties of $P(VDF/TrFE)$ and $BaTiO_3$ by local field and Monte Carlo computations — •Markus Kühn and Herbert Kliem — Saarland University, Institute of Electrical Engineering Physics, P.O. Box 151150, 66041 Saarbrücken, Germany.

For interacting model systems of the $P(VDF/TrFE)$ copolymer and the $BaTiO_3$ crystal dynamic Monte Carlo simulations are performed. The systems consist of field-induced point dipoles and permanent dipoles / ions. Both ferroelectric systems are placed between two coplanar conducting electrodes. All electrostatic interactions are considered and the electrodes are described by the method of images. The permanent dipoles / ions fluctuate thermally activated in double well potentials according to the Boltzmann statistics. The long-range electrostatic interactions strongly influence the local fields at the dipoles / ions. The iterative algorithm consists of two steps. For each current configuration the local fields at the dipoles / ions are deterministically calculated. Then the transition times of the dipoles / ions which depend on the local electric fields are computed in a following weighted probabilistic Monte Carlo step. As the main result we find ferroelectric hysteresis loops and polarisation switching curves. Further results for $P(VDF/TrFE)$ have shown that dielectric layers adjacent to the electrodes have an impact on the hystereses. Simulations of the (2 0 0)-plane for $BaTiO_3$ show a pronounced domain growth starting at the electrode. Snapshots of the system at different times further revealed a pronounced pinning effect at a discontinuity modelled by a vacancy.

DF 11.8 Wed 16:20 EB 107

Probing ferroelectricity in ultrathin wedged epitaxial $BaTiO_3$ films — •Adrian Petraru[1], Hermann Kohlstedt[1], Axel Solbach[2], Nikolay Pertsev[3], Uwe Klemradt[2], Willi Zander[4], Jürgen Schubert[4], and Rainer Waser[1] — [1]Institut für Festkoerperforschung und CNI, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]II. Physikalisches Institut B, RWTH Aachen University, 52074 Aachen, Germany — [3]A. F. Ioffe Physico-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [4]Institut für Bio - und Nanosysteme und CNI, Forschungszentrum Jülich GmbH, Jülich, Germany

High quality epitaxial wedged $BaTiO_3$ ultrathin films were grown epitaxially on $SrRuO_3$-covered (001) - oriented $SrTiO_3$ substrates by high-pressure sputtering. The composition along the wedge was checked by Rutherford Backscattering Spectrometry (RBS). The thickness slope and the in-plane and out-of plane lattice parameters of the wedge were studied by x-ray diffraction using a laboratory source and synchrotron radiation. The $BaTiO_3$ films were fully strained by the substrate. Ferroelectric capacitors were then fabricated from $SrTiO_3/SrRuO_3/BaTiO_3$(wedge)$/SrRuO_3$/Pt heterostructures using optical lithography and ion beam etching. Direct evidence of ferroelectricity in these films down to the thickness of 4 nm was obtained by measurements of polarization-voltage hysteresis loops.

DF 11.9 Wed 16:40 EB 107

A combined first principles and electron-holographic aproach to domain boundaries in (multi)ferroic materials — •Axel Rother[1], Nicola Spaldin[2], and Hannes Lichte[1] — [1]Institute for Structural Physics, TU Dresden, 01062, Germany — [2]Materials Department, University of California, Santa Barbara, CA 93106

Domain boundaries in ferroic materials deviate from the bulk in both the structural and electronic properties. Their presence in the material influences the total energy of the system as well as the dynamic properties, for instance during polarization switching. We report on a combined Density Functional Theory and Electron Holographic approach on domain boundaries in multiferroic $BiFeO_3$, ferroelectric $BaTiO_3$ and other (multi-)ferroic materials. Our model systems extend over different domain walls with respect to material composition and angular change and encompass between 50-120 atoms. The calculations were performed within VASP, a package for DFT using pseudopotentials and a plane wave basis set, particularly suited for such big systems. The calculations reveal the details of charge and structure modulation on the boundary, including the formation of dipole layers

and a change in the magnetic behaviour in case of $BiFeO_3$. Electron holographic measurements support the findings of the calculations by measuring dipole layers and charge modulations on the domain boundaries.

DF 12: Dielectric and ferroelectric thin films and nanostructures II

Time: Thursday 10:00–13:00 Location: EB 107

Invited Talk DF 12.1 Thu 10:00 EB 107

Piezoelectric ceramic materials - a success story — •Dieter Sporn[1], Andreas Schönecker[2], Bernhard Brunner[1], and Horst Beige[3] — [1]Fraunhofer-Institut fuer Silicatforschung, Neunerplatz 2, 97082 Wuerzburg — [2]Fraunhofer-Institut fuer Keramische Technologie und Systeme, Winterbergstrasse 28, 01277 Dresden — [3]Martin-Luther-Universität Halle-Wittenberg, Institut fuer Physik, Friedemann-Bach-Platz 6, 06108 Halle

The development of piezoelectric ceramic materials in the last decade offered a huge number of new applications. This can be shown by market numbers: the world wide market volume doubled from 2001 to 2006! This was driven by growing demands concerning of precise controls of structures and components, monitoring and adaptive systems, control of ignition points in engines, etc.

The success of the piezoelectric ceramics is based by tremendous efforts in material design, new compositions and new shaping opportunities. Beside commonly used buld materials it is evident, that piezoelectric films and fibers opened new applications. The development and the understandig of such structures is based on close cooperations between chemists, material scientists, physicists and engineers. One of the recently important issues is the search of new, lead-free compositions with properties similar to them of so far used lead-containing compositions.

In this contribution the efforts of the last years will be demonstrated on the hand of selected isssues (piezoelectric films, piezoelectric fibers and new compositions).

DF 12.2 Thu 10:40 EB 107

Thickness dependence of leakage current through capacitor stacks with high-k materials for DRAM application — •Herbert Schroeder — IEM im Institut für Festkörperforschung und CNI, Forschungszentrum Jülich GmbH, D-52425 Jülich

According to the International Technology Roadmap for Semiconductors (ITRS) the implementation of high-permittivity thin insulating films as dielectrics in capacitors (charge-based memory) and gates (MOSFET) is indispensable within the near future to achieve the documented goals. One of the most important issues for these applications is the sufficiently low leakage current through the metal/insulator/metal (MIM) capacitor stacks. A large number of experimental data on leakage current through MIM thin film capacitor structures is published for high-k perowskite-type mixed oxides, especially for the model alloys $SrTiO_3$ (STO) and (Ba,Sr)TiO_3 (BST). The mechanistic interpretation of these data is rather contradictory and therefore unsatisfactory. This especially holds for the current dependence on dielectric thickness, for which very different and opposite trends have been observed. This contribution reports simulation results of leakage curves within a new model combining current injection/ejection at the interfaces with drift-diffusion current in the film bulk with special emphasis on dielectric thickness. The main result is that the used model is able to describe all kinds of thickness dependencies as the current is dependent on the defect properties in the dielectric, i.e. type (donor and/or acceptor), densities, energy level in the gap, and type and degree of compensation (ionic, electronic), as well as electrode/interface properties.

DF 12.3 Thu 11:00 EB 107

Leakage spot evolution in thin $(ZrO_2)_{0.8}(Al_2O_3)_{0.2}$ -films observed by conductive atomic force microscopy (CAFM) — •Dominik Martin[1], Oliver Bierwagen[2], Matthias Grube[1], Lutz Geelhaar[2], and Henning Riechert[2] — [1]namlab gGmbh, D-01187 Dresden — [2]Qimonda, D-81730 Munich

A change from amorphous to nanocrystalline dielectric layers is necessary to achieve dielectric constants >30 as required for future technology nodes. This often leads to significantly higher leakage currents. These were measured in such inhomogeneous samples with a spatial resolution on the nanoscale. CAFM was used to characterize 20 nm-thin $(ZrO_2)_{0.8}(Al_2O_3)_{0.2}$ -films grown by molecular beam deposition. In nanocrystalline samples, there are hillocks at the surface with typical diameters and heights of 30 nm and 3 nm, respectively. An investigation by transmission electron microscopy implies that these hillocks are crystallites that protrude from the surface. CAFM current maps show leakage spots in which the current is significantly higher than in the surrounding matrix. These leakage spots are strongly correlated with the hillocks on the corresponding morphology images, indicating that the formation of crystallites really leads to leakage paths. To distinguish between different transport mechanisms, multiple images of the same area were taken, while the bias-voltage was changed consecutively. By using the entire set of images, IV-curves can be assigned to each location. These show a hysteretic behaviour for all leakage spots. Also, the voltage at which the strong increase in current occurs varies significantly for different leakage spots, i.e. between -1 V and -4 V.

DF 12.4 Thu 11:20 EB 107

The influence of image potential on defect assisted leakage mechanisms — •Grzegorz Kozlowski and Jarek Dabrowski — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

We present the results of numerical simulation of tunneling current through a dielectric film. A carrier inside a dielectric film between metallic plates encounters an additional potential resulting from the interaction with its electrical image in the metal. As a result not only the height of barrier is lowered and the bands are bent downwards in vicinity of the metal electrodes, but also the tunneling length is shortened. Besides causing the well-known Schottky effect, this increases the tunneling leakage. Maybe more interestingly, also leakage due to the presence of defects is affected. This is because carriers must be supplied from the electrode to the defect states. Without the image force, in many cases this supply process limits the current that may flow through defects. This limitation may be partially or completely lifted when the image force is taken into account. The image potential lowers both the energy of defect states in vicinity of the electrode and the energy barrier separating these defects from the electrode. We investigate the influence of this effect on the magnitude of leakage current for various leakage mechanisms including trap assisted tunneling and Poole-Frenkel conduction.

DF 12.5 Thu 11:40 EB 107

The mechanisms of leakage current in $BaHfO_3$ films — •Grzegorz Kozlowski, Jarek Dabrowski, Grzegorz Lupina, Gunther Lippert, Piotr Dudek, and Hans-Joachim Müssig — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

We present the results of theoretical and experimental study of leakage currents through ultrathin dielectric $BaHfO_3$ films in MIM (Metal-Insulator-Metal) capacitor structures. Ab initio calculations have been performed for defects and impurities, and standard electrical measurements have been done in order to reveal the physical processes governing the transport of charge carriers across the film. The dominating leakage mechanism clearly depends on temperature, voltage, and film thickness. Statistical analysis of leakage currents provides further information on the character of the responsible defects, e.g., allowing us to attribute the leakage at given conditions to microscopic or macroscopic defects. We confront the results of this experimental data analysis with the ab initio data and we discuss the implications on the film deposition and processing.

DF 12.6 Thu 12:00 EB 107

On the electronic and dielectric characterisation of thin cubic PrO_2 layers on Silicon — •Olaf Seifarth[1], Christian Walczyk[1], Grzegorz Lupina[1], Jaroslaw Dabrowski[1], Günter Weidner[1], Peter Zaumseil[1], Dieter Schmeisser[2], Peter Storck[3], Hans-Joachim Müssig[1], and Thomas Schroeder[1] — [1]IHP microelectronics, 15236 Frankfurt (Oder), Germany — [2]Brandenburg Technical University, 03046 Cottbus, Germany — [3]Siltronic AG, 81737 München, Germany

For the integration of 100 % Ge onto the Si platform, a buffer oxide ap-

proach has been developed recently, using rare earth oxides to tune the lattice constant between the Si and the Ge. Among these buffer oxides, PrO_2 is a prospective candidate with high quality crystalline growth on Si, moderated by an interfacial Pr-silicate between. In order to specify electronic properties of thin PrO_2 and its interface on Si(111), especially the width of the band gap, we performed synchrotron radiation based XPS, UPS and XAS measurements at the U49/2 PGM 2 beamline at BESSY II and correlate the results with our structural characterisation performed by TEM and XRD. In order to evaluate the dielectric properties of thin PrO_2 layers on Si(111), we performed temperature-, time-, voltage-, and layer thickness-dependent leakage current measurements (J-V). Here, we identified relaxation behaviour in the leakage current, successfully addressed to defect like states inside the Pr-silicate interface layer, corroborated by frequency dependent capacitance versus voltage (C-V) measurements.

DF 12.7 Thu 12:20 EB 107

Transition metal oxide based NVM for IHPs 0.13 micron BiCMOS technology — •Rakesh Sohal, Christian Walczyk, Ioan Costina, Peter Zauseil, Alexander Fox, and Thomas Schroeder — IHP Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

This Research is targeted to increase the functionality of IHP's 0.13 micron BiCMOS technology by integrating innovative embedded NVM cell concepts. The material of our interest is the tungsten oxide as insulator in metal-insulator-metal (MIM) structure to develop so called back-end-of-line (BEOL) integrated OxRAM cells. In this study, we report on the investigation of the tungsten oxidation process under BEOL constraints (<450°C) by using XPS, XRD, XRR and SEM.

The CVD prepared tungsten layers on TiN covered silicon wafers are thermally oxidised in oxygen environment (with 200 sccm O2 flow rate) in the temperature range of 300-450°C for 15-75 minutes. The tungsten oxide layer thickness estimated by XRR was in the range of 6 nm to 80 nm. The tungsten oxide was in WO3 stoichiometry as confirmed by XPS. The tungsten oxide prepared at higher temperatures (>350°C) show a small shoulder at lower binding energy which corresponds to tungsten sub-oxides. The tungsten oxide starts to crystallise in monoclinic phase at 350°C when it is oxidised for 30 minutes. A (001) oriented growth texture becomes dominant at higher temperatures (>400°C). The tungsten oxide surface was uniform for the layers prepared below 400°C. The tungsten oxide layers were also characterised by analysing the dielectric behaviour (i.e. leakage current).

DF 12.8 Thu 12:40 EB 107

Space charge polarization in solid electrolytes — •Björn Martin and Herbert Kliem — Saarland University, Germany

Thin films of polyethylene oxide are investigated as model systems for a solid electrolyte. Plane parallel capacitance structures of these samples show a pronounced relaxational behaviour with a thickness dependent effective dielectric constant in the low frequency range. This behaviour is attributed to a space charge polarization of mobile ions in the material.

With a three-dimensional discrete hopping model, it is possible to describe the dielectric properties of the systems. Here, mobile charges can fluctuate thermally activated over barriers in a multiwell energy structure. If all interactions in the system, especially the attracting interactions between the ions and their image charges in the electrodes, are considered, it can be shown that electrode effects play an important role. Thus, these effects are responsible for a Kohlrausch behavior of the polarization current in the long time range as well as for an increased accumulation of charges at the electrodes.

The space charge distribution, predicted by simulations of the model system, is determined by measurements of the surface potential with a scanning Kelvin probe contactless [1]. Due to the motion of negative mobile ions after application of an electric field a positive space charge region is found near the negative electrode resulting in a strongly nonlinear surface potential. Additionally a charge injection process is observed.

[1] B. Martin, H. Kliem, acc. by IEEE Trans. Dielectr. Electr. Insul.

DF 13: Dielectric and ferroelectric thin films and nanostructures III

Time: Thursday 14:00–17:00 Location: EB 107

DF 13.1 Thu 14:00 EB 107

Current transport mechanism in metal/HfO_2/metal structures — •christian walczyk[1], thomas schroeder[1], christian wenger[1], jaroslaw dabrowski[1], mindaugas lukosius[1], sergej pasko[2], and christoph lohe[2] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — [2]AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany.

The metal-insulator-metal (MIM) capacitor integration into BiCMOS technology is governed by the efforts toward increasing the capacitance density, reducing the leakage current density and improving the voltage linearity. In particular, achievement of an acceptable leakage current density in BEOL MIM capacitors is still a challenge. To get around this critical problem, high-k dielectrics have been introduced. Among various candidates, HfO_2 has been investigated due to its high dielectric constant, low leakage current and chemical stability [1]. Despite the considerable efforts for HfO_2, its current transport mechanism in MIM structures needs further investigations. Based on experimental results of the temperature dependence of the leakage current, we studied the current transport mechanism and energy band diagrams. The leakage current was measured in the temperature range of 200 - 400 K. The slope of an Arrhenius plot yielded activation energies in the range of $E_a = 0.2$ eV. In particular, we obtained a trap level at $\phi_{PF} = 0.4$ eV below the HfO_2 conduction band which contributes to Poole-Frenkel conduction.

[1] M. Houssa et al., Materials Science and Engineering R51, (2006).

DF 13.2 Thu 14:20 EB 107

Characterisation of thin tantalum oxide films — •Katrin Bruder[1], Achim Walter Hassel[1], and Detlef Diesing[2] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf — [2]Institut für physikalische Chemie, Universität Duisburg-Essen, 45141 Essen

Metal-Insulator-Metal (MIM, consisting of tantalum– anodic tantalum oxide–platinum) contacts were investigated by means of IV characteristics and impedance spectroscopy. With impedance spectroscopy it is possible to determine the capacitance, the metals resistivities and the tunnel resistance. The latter one is a function of the bias voltage, while the capacitance and metals resistivities remain constant. The tunnel resistivity was found to have a maximum at a bias U_{max} slightly different from 0 V. This shift was investigated as a function of the film thickness (d = 4 nm to 12 nm) and the temperature in the range from $T = 58$ K to 350 K. The measurements were compared to simulations. These simulations show, that for an explanation of this shift, asymmetrical barriers and tunneling through the valence band has to be considered.

DF 13.3 Thu 14:40 EB 107

Hyperfeinwechselwirkung in dünnen Schichten von HfO_2 — •Michael Steffens[1], Reiner Vianden[1] und Andre Stesmans[2] — [1]Helmholtz - Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn, Germany — [2]Dept. of Physics, Celestijnenlaan 200D, 3001 Leuven, Belgium

Das „high-κ"-Dielektrikum HfO_2 soll als Nachfolger von SiO_2 als Gate-Oxid in MOSFET-Strukturen eingesetzt werden. In dieser Technologie gefertigte Chips haben bereits Marktreife erreicht. Durch diesen Übergang wird der Weg für eine weitere zukünftige Leistungssteigerung im Sinne des Mooreschen Gesetzes ermöglicht. Zwar wurde HfO_2 in den vergangenen Jahren intensiv studiert, vollständig verstanden sind seine Eigenschaften jedoch nicht.

Die Hyperfeinwechselwirkung des Hf in 100 nm dünnen Schichten HfO_2 wurde mit der gestörten $\gamma-\gamma$-Winkelkorrelation (PAC) untersucht. Die PAC eignet sich besonders für die Bestimmung der lokalen Umgebung eines Sondenkerns im Material. Die PAC-Sonde ^{181}Hf wird durch Neutronenaktivierung des natürlich in den Proben vorkommenden ^{180}Hf erzeugt. Die Filmproben sind mit ALCVD und MOCVD auf einem einkristallinen (100)Si-Substrat gewachsen.

An verschieden thermisch behandelten Proben wurden PAC-Messungen durchgeführt. Die Ergebnisse eines isochronen Ausheilpro-

gramms und temperaturabhängiger Messungen werden gezeigt und im Vergleich zum Verhalten von gleichbehandeltem reinem HfO_2 diskutiert. Schwerpunkt ist dabei die Kristallstruktur der Schichten und ihr Verhalten unter Temperatureinflüssen.

DF 13.4 Thu 15:00 EB 107

Atomic vapour deposition of Sr-Ta-O films for MIM applications — •Mindaugas Lukosius[1], Christian Wenger[1], Sergej Pasko[2], Ioan Costina[1], Jaroslaw Dabrowski[1], Roland Sorge[1], Hans-Joachim Müssig[1], and Christoph Lohe[2] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]AIXTRON AG, Kackertstr. 15-17, 52072 Aachen, Germany

Metal-Insulator-Metal (MIM) capacitors are widely used in ICs for Radio-Frequency (RF) applications. Advanced RF-technologies require further reduction in feature size combined with several significant materials challenges: according to the International Roadmap for Semiconductors for wireless communication technologies, the capacitance density should be higher than 5 fF/*m2, capacitance variation and leakage current should be minimized and quality factor should be maximized [1]. These requirements imply the replacement of silicon oxide-based dielectrics with new high-k materials. Sr-Ta-O thin films are of interest for applications as high-k dielectric in MIM capacitors in CMOS back-end of line (BEOL) due to their high permittivity.

Depositions of strontium tantalate films were performed by Atomic Vapor Deposition (AVD) technique. We observed that the process pressure has a considerable influence on the stoichiometry of the deposited Sr-Ta-O films as well as on some electrical properties.

[1] RF and Analog/Mixed-Signal Technologies for Wireless Communications, ITRS (Semiconductor Industry Association, Palo Alto 2006 update).

DF 13.5 Thu 15:20 EB 107

Surface preparation of TiN electrodes for subsequent HfO2-based high-k dielectrics deposition. — •Peter Dudek, Grzegorz Lupina, Thomas Schroeder, and Hans-Joachim Muessig — IHP-Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder) / Germany

High-k dielectrics combined with compatible metal electrodes are significant material research approaches to scale down dynamic random access memories (DRAM). Accordingly, TiN-based electrodes require strict control of the surface chemistry to avoid the presence of performance limiting interfacials1. Recent studies show an interfacial layer present on the TiN electrode forming TiN/TiONx/TiO2 materials stack. Different etching methods for interface removal have been applied and characterised by x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM). Direct comparison of high-k dielectric properties on treated and as-deposited TiN electrode is the objective of research.

[1] Schroeder et al. J.Appl.Phys. 102, (2007).

DF 13.6 Thu 15:40 EB 107

Growth of HfO_x thin films by reactive molecular beam epitaxy — •Erwin Hildebrandt, Jose Kurian, and Lambert Alff — Institut für Materialwissenschaft, TU Darmstadt

Thin films of hafnium oxide were grown on single crystal r-cut and c-cut sapphire by reactive molecular beam epitaxy. The conditions for the growth of single oriented hafnium oxide thin films have been established. Hafnium oxide thin films were characterized by x-ray diffraction and optical absorption measurements. It was found that hafnium oxide thin films grown on r-cut sapphire were (00l) oriented whereas, on c-cut sapphire, hafnium oxide films showed different orientations depending on the growth temperature and oxidation conditions. The hafnium oxide films grown at higher temperature and under strong oxidation conditions yielded (00l) oriented films on c-cut sapphire whereas slightly weaker oxidation condition leads to (111) oriented hafnium oxide films. The bandgap deducted from optical absorption measurement carried out on hafnium oxide films grown under optimized conditions agreed well with the values reported in literature. A range of oxygen deficient thin films of hafnium oxide were also grown on single crystal sapphire substrates in order to investigate the effect of oxygen vacancies on dielectric properties of hafnium oxide. The oxygen deficient thin films of hafnium oxide show a decrease in bandgap with increase in oxygen deficiency.

DF 13.7 Thu 16:00 EB 107

Investigation of $(SrO)_x(ZrO_2)_{(1-x)}$ high-k dielectrics deposited by molecular beam deposition — •Matthias Grube[1], Oliver Bierwagen[2], Dominik Martin[1], Lutz Geelhaar[2], and Henning Riechert[2] — [1]namlab gGmbh, D-01187 Dresden — [2]Qimonda, D-81730 Munich

Thin high-k dielectrics will be essential for metal-insulator-metal capacitors in future dynamic random access memory. Focused on this necessity, we investigated thin amorphous films of ZrO_2 and $(SrO)_x(ZrO_2)_{(1-x)}$ grown by molecular beam deposition. As substrates, we used n^{++}-Si-wafers which were covered with a predeposited 5 nm-thin TiN layer. Current-voltage and capacitance-voltage measurements were performed to determine the electrical properties of the dielectrics.

The ZrO_2 films were grown by three different methods, either in ultra-high vacuum or with an additional supply of O_2, and employing either Zr or ZrO targets. A k-value of 23 - 28 was extracted from a thickness-series, which is consistent with the value for amorphous ZrO_2.

$(SrO)_x(ZrO_2)_{(1-x)}$ was grown by co-evaporating SrO and ZrO_2. For as-grown films with $x \approx 0.6$, a k-value of about 6 was extracted. This is significantly lower than the tabulated value. Preliminary experiments for $x \approx 0.4$ indicate a more reasonable value of $k \approx 20$. In addition, post-deposition annealing experiments were performed, which improved the properties of the films. Their density was increased, and their capacitance equivalent thickness was reduced to 50% and less.

DF 13.8 Thu 16:20 EB 107

Computer-simulated Fullerene-based dielectric materials: Ways to improve the properties of the generated ultralow-k structures — •Kostyantyn Zagorodniy, Helmut Hermann, and Manfred Taut — Leibniz Institute for Solid State and Materials Research, IFW Dresden, PF 270116, D-01171 Dresden, Germany

Insulating low-k dielectric materials are needed to minimize cross-talk between metal interconnects in microelectronic products. The continuous shrinking of device dimensions of ultra-large-scale integrated (ULSI) chips imposes strong demands on the backend of the line (BEoL) interconnect structures. The International Technology Roadmap for Semiconductors (ITRS) indicates that the k values need to be reduced to 2.0 for the 45 nm technology node or bellow in the next few years. Additionally to extremely low dielectric constants, new insulating materials must have also suitable mechanical properties. We have recently proposed the model for new ultralow-k dielectrics as an ordered three-dimensional network consisting of two components: C60 Fullerenes as nodes and bridge molecules as edges connecting the nodes. In the present work we analyze the generated structures in order to improve mechanical and electronic properties. Substituting of the bridge molecules and varying the ways of connecting them to the C60 molecule the mechanical and electronic properties of the model can be affected. Classical and quantum-chemical methods are used to optimize the structures and to calculate its properties. Possible improvements and the limitations are discussed.

DF 13.9 Thu 16:40 EB 107

Molecular Beam Epitaxy of crystalline oxides on Si for C-MOS and for the monolithic integration of semiconductors on Silicon — •Guillaume Saint-Girons[1], Clément Merckling[1], Mario El-Kazzi[1], Loic Becerra[1], Philippe Regreny[1], Gilles Patriarche[2], ludovic Largeau[2], Vincent Favre-Nicolin[1], and Guy Hollinger[3] — [1]INL/UMR5270, site ECL, 36 av. Guy de Collongue, 69134 Ecully cedex, France — [2]LPN-UPR20/CNRS, Route de Nozay, 91460 Marcoussis, France — [3]CEA/DRFMC/SP2M, 17 rue des Martyrs 38054 Grenoble and UJF, BP53, 38041 Grenoble cedex 9, France

In this contribution, a detailed description of the growth mechanisms and structural properties of high-k Al_2O_3, Gd_2O_3 and amorphous $LaAlO_3$ on Si will be presented. On the basis of these studies, relevant oxide/Si systems will be proposed that fulfill the requirements of future C-MOS systems. In particular, very promising electrical characteristics have been obtained showing that the (amorphous $LaAlO_3$)/Si system is compatible with ITRS recommendations in terms of EOT and leakage current. Moreover, it will also be shown that InP/oxide heterointerfaces present a quasi-ideal compliant behavior that opens the way to the monolithic integration of III-V heterostructures on Si for advanced micro and optoelectronic applications.

DF 14: Electric, electromechanical and optical properties II

Time: Thursday 14:00–17:20 Location: EB 407

DF 14.1 Thu 14:00 EB 407

Consequences of hopping charge transport for the relaxation of light-induced absorption in oxide crystals — •Christoph Merschjann, Bettina Schoke, and Mirco Imlau — Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück

Transient light-induced absorption changes $\alpha_{\mathrm{li}}(t)$ are observed in various nonlinear optical oxide crystals as, e.g., $LiNbO_3$, $KNbO_3$, $KTiOPO_4$, and β-BaB_2O_4. In contrast to basic assumptions the decay shape of $\alpha_{\mathrm{li}}(t)$ in these materials is generally not monoexponential. A fairly good — though empirical — description of the temporal evolution of the light-induced absorption is given by stretched exponential functions: $\alpha_{\mathrm{li}}(t) = \alpha_{\mathrm{li}}^{(0)} \cdot \exp\left[-(t/\tau)^{\beta}\right]$, with $0 < \beta \leq 1$. However, the origin of this peculiar behavior is still unclear. One possible reason may be a random-walk hopping transport of excited charge carriers, as predicted by the theory for small polarons in oxide crystals.

We present random-walk simulations of both band and hopping charge transport with different complexities. The results indicate that hopping transport is more likely to lead to the observed effects than classical band transport. The connection between transport models and mathematical descriptions of $\alpha_{\mathrm{li}}(t)$ is discussed.

Supported by the Deutsche Forschungsgemeinschaft (Projects IM 37/2-2, TFB 13-04, and GRK 695).

DF 14.2 Thu 14:20 EB 407

Absorption of ultra-short laser pulses in dielectrics — •Stefan Linden and Bärbel Rethfeld — TU Kaiserslautern

If an insulator is irradiated by a laser pulse of sufficient high intensity, non-linear ionization processes lead to an increasing free-electron density in the conduction band of the insulator. Free electrons enhance the absorptivity of the initially transparent material and are responsible for the optical breakdown of dielectrics. The transient free electron density is a fundamental parameter for numerous theoretical and experimental investigations and applications.

To describe the transient electron density in the dielectric several models exist. Commonly, a simple rate equation is applied to describe the evolution of the free-electron density under laser irradiation. Though this equation is proved for nano- to picosecond time scales, it fails on ultra-short processes. Here, the electrons energy distribution has to be taken into account, for example in the frame of the multiple rate equation [1].

In this study we present an extension of the multiple rate equation, taking into account the recombination of excited electrons from the conduction band to exciton states. Such exciton recombination was experimentally found to occur within about 200 fs for the case of SiO_2. We introduce the recombination time phenomenologically in the multiple rate equation and seek for an analytical asymptotic solution, giving information about the applicability of different approaches.

[1] B. Rethfeld, *Phys. Rev. Lett.* **92**, 187401, (2004).

DF 14.3 Thu 14:40 EB 407

Light-induced absorption in electrooptic PLZT ceramics — •Torsten Granzow[1], Silke Schaab[1], Dominik Schaniel[2], and Theo Woike[2] — [1]FB Material- und Geowissenschaften, TU Darmstadt, Germany — [2]Institut für Mineralogie, Universität zu Köln, Germany

Transparent polycrystalline materials such as lanthanum-modified lead-zirconate-titanate ceramics (PLZT) have electrical and electrooptical properties that can rival those of single crystals such as lithium niobate (LNB). At the same time, they offer all the advantages of ceramics, e.g. quick and cheap production in nearly arbitrary shape and size. However, there has been hardly any investigation of light-induced changes of the optical properties of PLZT such as its photorefractive behavior or light-induced changes of the optical absorption.

In this talk, we present measurements of the light-induced absorption in PLZT containing 8% La, 65% Zr and 35% Ti (PLZT 8/65/35). The samples are illuminated by a pulse from a Nd:YAG-laser, the resulting absorption change is detected by measuring the intensity of a probe laser behind the sample. A strong light induced absorption is detected in a broad spectral range. Its temporal development strongly depends on the probing wavelength: at high wavelengths there is a continuous decrease, lower wavelengths show an increase of the absorption for several microseconds before this absorption also finally subsides. This effect is attributed to the presence of two different electronic centers in the band gap. The results are discussed in comparison to LNB single crystals and with respect to possible photorefractive applications.

DF 14.4 Thu 15:00 EB 407

Space-charge waves of the low-frequency branch with a linear dispersion law — •Michaela Lemmer[1], Mirco Imlau[1], Manfred Wöhlecke[1], Mikhail P Petrov[2], and Konstantin Shcherbin[3] — [1]Department of Physics, University of Osnabrück, Osnabrück, Germany — [2]Ioffe Physico Technical Institute, St. Petersburg, Russia — [3]Institute of Physics, National Academy of Sciences, Kiev, Ukraine

ac and dc currents arising in CdTe:Ge during optical excitation of space-charge waves (SCW) have been investigated. The experiments have been performed at a wavelength of $\lambda = 1064$ nm using the technique of an oscillating interference pattern. Our investigations have shown that the SCW studied can be attributed unambiguously to trap recharging waves (TRW). Remarkably, we have found a linear dispersion law ($\Omega_K \sim K$) for these waves although an inverse law is usually expected. A corresponding theoretical model has been developed and shows that the theoretical data are in reasonable agreement with the experiments if the following fitting parameters are used: An effective trap concentration of $N_{\mathrm{eff}} = (2.5 \pm 0.3) \cdot 10^{12}$ cm^{-3}, a mobility-lifetime product of $\mu\tau = (0.65 \pm 0.05) \cdot 10^{-7}$ cm^2/V, and a Maxwell relaxation time of $\tau_M = (5.5 \pm 0.2) \cdot 10^{-3}$ s. The appearance of an additional low-frequency ac resonance is discussed in the frame of a bipolar conductivity.

Financial support of the Deutsche Forschungsgemeinschaft (DFG, projects GRK 695 and RUS 17/15/07) is gratefully acknowledged.

DF 14.5 Thu 15:20 EB 407

Untersuchung des photorefraktiven Effekts in Lithiumniobat-Kristallen mit Femtosekunden-Laserpulsen* — •Dominik Maxein, Stephan Kratz, Daniel Haertle und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Der sogenannte photorefraktive (PR) Effekt spielt bei vielen Anwendungen von Lithiumniobat-Kristallen ($LiNbO_3$) eine wichtige Rolle: Einerseits kommt es durch Brechungsindexänderungen bei hohen Intensitäten zum „optischen Schaden“, durch den das Strahlprofil zerstört wird. Andererseits bietet er die Möglichkeit, Brechungsindexstrukturen und diffraktive optische Elemente in $LiNbO_3$ einzuschreiben, aber bisher im Wesentlichen nur mit sichtbarem Licht.

Kürzlich wurde mit Einstrahlexperimenten gezeigt, dass der PR Effekt in $LiNbO_3$:Fe auch bei Licht der Telekommunikationswellenlänge 1,5 μm auftritt, wenn man fs-Pulse verwendet [1]. Allerdings zeigt er dort Besonderheiten: Man erreicht vergleichsweise hohe Brechungsindexänderungen Δn und beobachtet einen Vorzeichenwechsel des Δn-Musters beim Wechsel der Schreiblicht-Polarisation. Um den PR Effekt sowie diese Besonderheiten besser zu verstehen, wird das Schreiben und Löschen von Gittern in $LiNbO_3$ mit fs-Laserpulsen untersucht und mit cw-Messungen verglichen. Dabei kommt sichtbares (532 nm) und infrarotes Licht (776 nm) zum Einsatz.

* Gefördert von der DFG und der Deutschen Telekom AG.

[1] O. Beyer et al.: "Photorefractive effect in iron-doped lithium niobate crystals induced by femtosecond pulses of 1.5 μm wavelength," Appl. Phys. Lett. 88, 051120 (2006)

DF 14.6 Thu 15:40 EB 407

Polungsverhalten und Brechungsindex in magnesiumdotiertem Lithiumniobat nach Bestrahlung mit hochenergetischen Ionen — •Lena Jentjens[1], Hilke Hattermann[1], Konrad Peithmann[1], Matz Haaks[1], Karl Maier[1] und Michael Kösters[2] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn — [2]Physikalisches Institut, Universität Bonn

Mit Magnesium dotiertes Lithiumniobat ($LiNbO_3 : Mg$) ist auf Grund des stark unterdrückten photorefraktiven Effekts für viele Anwendungen interessant. Durch die Bestrahlung mit leichten, hochenergetischen Ionen wie ^{3}He mit einer Energie von 41 MeV werden wichtige Materialeigenschaften geändert. In der bestrahlten Region, in der die Ionen den Großteil ihrer Energie noch nicht abgegeben haben (vor dem Bragg-Peak), ist das ferroelektrische Koerzitivfeld E_C um 0.6 bis 1.0 kVmm^{-1} vermindert. Das Umpolen von Domänen in bestrahl-

ten Bereichen wird so im Vergleich zu unbestrahlten Bereichen entscheidend erleichtert. Außerdem werden im Kristall thermisch stabile Brechungsindexänderungen in der Größenordnung 6×10^{-3} durch die Bestrahlung verursacht. Diese Eigenschaften sind besonders im Bereich der kleinräumigen Strukturierung interessant, die unter anderem bei Anwendungen in der nicht-linearen Optik eine große Rolle spielt. (*gefördert durch DFG-FOR 557)

DF 14.7 Thu 16:00 EB 407

UV-assisted electrical field poling of magnesium-doped lithium niobate crystals* — •Hendrik Steigerwald, Fabian Luedtke, and Karsten Buse — Institute of Physics, University of Bonn, Wegelerstraße 8, 53115 Bonn, Germany

Periodically-poled lithium niobate ($LiNbO_3$) with domain structures in the micrometer regime is intensively investigated due to its increasing importance, e.g. for nonlinear optics using quasi phase matching. Efficient second harmonic generation in this material is usually hampered by optical damage, i.e. undesired index and absorption changes. Mg-doping increases the optical damage threshold, however complicates the poling process especially for small domain structures. We obtain such domain patterns in Mg:$LiNbO_3$ crystals by a combined approach using electric field poling and a superimposed UV light grating. Illumination with UV light decreases the coercive field of Mg:$LiNbO_3$ and enables smooth domain wall propagation. Structured coating of a z-cut Mg:$LiNbO_3$ crystal with UV-absorbing photoresist that has high electrical resistance enables electrical pulse poling of domain structures. The resulting domain patterns are investigated for different types of crystals and different poling parameters. Using this approach we also fabricated surface domains in proton exchanged α-phase waveguides.

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Self-induced fixing of index gratings in $LiNbO_3$:Fe using a single laser beam — •Volker Dieckmann, Andreas Selinger, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Self-induced fixing of noisy refractive-index gratings is discovered in single crystals of iron-doped $LiNbO_3$ (0.1 wt.% Fe) upon long-term exposure to a single laser beam of high intensity ($I = 100$ W/cm^2) at ambient temperature. The extraordinary polarized laser beam ($\lambda = 532$ nm) impinges normal to the c-axis of the sample. At the beginning of exposure, this results in the recording of noisy refractive-index gratings and in a nearly symmetric angular intensity distribution in $\pm c$-direction of scattered light (Goulkov et al., Phys. Rev. B, 65, 195111 (2002)). Further exposure to the high intense laser beam leads to a decrease of the scattered light intensity and, on the long-term, to an increase of an asymmetric scattering intensity distribution in $-c$-direction only. This distribution cannot be erased by white-light exposure, i.e. the underlying noisy refractive-index gratings are permanently fixed. Temperature-dependent measurements of the thermally activated decay of the gratings yield an activation energy of (0.97 ± 0.06) eV, which points to a contribution of charge-carriers with a low mobility, such as ions. The experimental procedure and the measured activation energy suggest an explaination via the effect of laser-induced local heating of the sample in combination with the well-known simultaneous thermal fixing procedure.

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DF 14.9 Thu 16:40 EB 407

Optical cleaning of lithium niobate crystals for reduction of optical damage* — •Michael Kösters[1], Patrick Werheit[1], Daniel Haertle[1], Karsten Buse[1], and Boris Sturman[2] — [1]Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany — [2]Institute of Automation and Electrometry, 630090 Novosibirsk, Russia

A method for the reduction of optical damage in lithium niobate crystals is presented: The crystals are illuminated with a focused laser beam giving rise to strong bulk photovoltaic electronic currents. At the same time, application of high temperatures of about 180 °C prevents the build-up of space charge fields by enhancing the mobility of ionic compensation charges, such as hydrogen ions. Experimentally, the method is similar to "thermal fixing" used for persistent hologram recording. Optimum choice of the light pattern plus heat however dramatically decreases the concentration of photoexcitable electrons in the exposed region leading to a suppression of optical damage. Experiments with slightly iron-doped crystals have shown an increase of the threshold for optical damage of more than 100 compared to untreated crystals. Crystals treated with this method could be of great use for non-linear optics, especially for applications using periodically-poled structures to enable quasi-phase matching: in contrast to magnesium doping for optical damage reduction, the method does not affect the good poling characteristics of undoped lithium niobate.

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A model for the thermo-electric oxidization of lithium niobate crystals* — •Stephan Gronenborn[1], Boris Sturman[2], Matthias Falk[1], Daniel Haertle[1], and Karsten Buse[1] — [1]Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany — [2]Institute of Automation and Electrometry, Novosibirsk 630090, Russia

Lithium niobate is an important material for many applications in optics e.g. electro-optic modulators, holography and frequency conversion. Using $LiNbO_3$:Fe, concentrations of Fe^{2+} and Fe^{3+} ions are important factors determining the performance of the material. Recently, a method to strongly oxidize highly doped crystals (0.5 - 3 wt.% iron in the melt), the thermo-electric oxidization treatment, was reported [1]. The crystals are annealed in the presence of an externally applied electrical field. The iron impurities are nearly completely oxidized to the Fe^{3+} state. The concentration of Fe^{2+} is decreased by 4 to 5 orders of magnitude, compared to less than one order achieved with conventional oxidization. The oxidization starts at the cathode and forms a sharp front, which moves through the crystal. A model for the charge migration in the crystal during the treatment based on a step profile of the Fe^{2+} concentration is developed. It is experimentally verified by spatially-resolved absorption measurements and in-situ investigations of the electric potential distribution inside the crystal and the oxidation front velocity at different temperatures and doping concentrations.

*supported by the Deutsche Telekom AG

[1] M. Falk and K. Buse, Appl. Phys. B **81**, 853 (2005)