DF 19: Poster 2

Time: Wednesday 15:00–17:30 Location: Poster B2

DF 19.1 Wed 15:00 Poster B2

The electronic structure of tetragonal CuO — •Simon Moser[1,2], Luca Moreschini[2], Davide Innocenti[2,3], Young Jun Chang[2,4], Aaron Bostwick[2], Eli Rotenberg[2], and Marco Grioni[1] — [1]Ecole Polytechnique Federale de Lausanne — [2]Advanced Light Source, Lawrence Berkeley National Laboratory — [3]University of Rome Tor Vergata — [4]University of Seoul

The cupric oxide CuO exhibits an insulating ground state with a correlation-induced charge-transfer gap and antiferromagnetism. It is, in principle, the most straightforward parent compound of the doped cuprates, and therefore has been theoretically studied as a model material for high temperature superconductivity.

Bulk CuO crystallizes in a low-symmetry monoclinic form, in contrast to the rocksalt structure typical of late 3d transition metal monoxides. It was recently synthesized by epitaxial growth on $SrTiO_3$ substrates in a higher symmetry tetragonal structure with elongated c-axis (Siemons *et* al. PRB 79, 2009). Extrapolating the behavior of other 3d transition metal monoxides, this phase of CuO is predicted to have a much higher Neel temperature than its bulk counterpart.

At beamline 7 of the Advanced Light Source, we have grown tetragonal CuO thin films by pulsed laser deposition and investigated their electronic structure by angle-resolved photoelectron spectroscopy (ARPES). These measurements represent the first mapping of the band structure of this new material, not available in bulk phase, and will serve as a reference point for future doping experiments.

DF 19.2 Wed 15:00 Poster B2

Free energy barriers of oxygen vacancy migration in TiO_2 — Michael Wehlau, •Jan Michael Knaup, and Thomas Frauenheim — BCCMS, Universität Bremen, Germany

To understand the memristive effect in reduced TiO_2, it is of supreme importance to understand the migration behavior of oxygen vacancy (V_O) defects in the material. A basic building block of this understanding are the free energy barriers of (V_O) migration and the influence of various external driving forces on these barriers. Previous results show that due to the immense dielectric constant of titania, the thermodynamic effect of external electric fields is very small even close to dielectric breakdown. However, since the ionic shifts causing this high permeability may influence the migration barriers, these must be analyzed in detail. We perform meta dynamics simulation of the migration of single (V_O) defetcs in rutile TiO_2, based on the Density-Functional based Tight-Binding (DFTB) method. To this end, we develop generally applicable collective variables that allow drive the dynamics of the vacancy rather than attempting to achieve this effect indirectly by driving surrounding atoms. Our results show that using the right kind of collective variables, meta dynamics is well suited to explore the migration mechanisms point defects in solids. Our findings on the free diffusion of (V_O) are in good agreement with previous results.

DF 19.3 Wed 15:00 Poster B2

Optical resonances of self-organized monocrystalline Au nanoparticles embedded in a $SrTiO_3$ matrix — •Hendrik Bernhardt[1], Christian Katzer[1], Christke Sandra[1], Frank Schmidl[1], Gabriele Schmidl[2], Wolfgang Fritzsche[2], Jörg Petschulat[3], Thomas Pertsch[3], and Markus Rettenmayr[4] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena, Germany — [2]Institute of Photonic Technology, IPHT, Albert-Einstein-Straße 9, D-07745 Jena, Germany — [3]Institut für Angewandte Physik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany — [4]Institut für Materialwissenschaft und Werkstofftechnologie, Friedrich-Schiller-Universität Jena, Löbdergraben 32

Gold nanoparticles in dielectric thin films are well known as plasmonically active material due to the excitation of localized surface plasmon resonances. Apart from the dielectric properties of the ambient medium and the inter-particle distances also shape and size of the particles can influence the resonance frequency. In this work, we report on ellipsoidal and orientated Au nanoantennas, which can be prepared in a crystalline high index ambient, i.e. $SrTiO_3$ (STO), via laser ablation. By controlling the deposition parameters, we are able to tune size, shape and distribution density of the crystalline gold nanoparticles. The plasmonic activity of the highly oriented nanoantennas thereby is observed in transmission spectroscopy experiments. Furthermore we will present transmission electron microscopy and x-ray diffraction data.

DF 19.4 Wed 15:00 Poster B2

Voltage-dependent impedance analysis of metal/ta-C/Si heterostructures — •Julian Alexander Amani, Tristan Koppe, Hans Hofsäss, and Ulrich Vetter — II. Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland

Whether tetrahedral amorphous carbon (ta-C) is used as electrode coating for electrochemical impedance spectroscopy (EIS) or as coating on medical implants, knowledge of its impedance properties is essential.

Different electrical equivalent circuits (EECs) have been proposed to reproduce the electrical properties of ta-C, so far, ignoring the knowledge of the voltage-dependence of its DC conductivity. Considering voltage-dependence of elements in an EEC facilitates correct assignment of circuit components to different parts of the investigated system and, hence, permits selection of the EEC with most accurate description of the underlying physics.

In this work, voltage-dependent impedance spectra were measured and compared to simulations, eliminating the ambiguity of the different proposed circuits. It could be shown that a Voigt-type circuit of a voltage-dependent resistance and a voltage-independent constant-phase element (CPE) describes the ta-C layer correctly. In contrast to most impedance analyses, the voltage- and frequency-dependence of the system was calculated and compared to the measured values in the complete parameter-space, not only for a single frequency spectra at each bias voltage separately. Possibility of large-signal analysis in time-domain allowed realistic simulations of the extremely non-linear resistive behaviour of ta-C.

DF 19.5 Wed 15:00 Poster B2

Tunable ferroelectric imprint and Mn valency in $PbTiO_3$ /$La_{0.7}Sr_{0.3}MnO_3$ nanostructures — •Ingo Krug[1], Ionela Vrejoiu[2,3], Alessio Morelli[2], Florian Nickel[1], Daniel Gottlob[1], Hatice Doganay[1], Robert Laskowski[4], Nick Barrett[5], Jiale Wang[5], and Claus M. Schneider[1,6,7] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, DE-52425 Jülich, Germany — [2]Max Planck Institut für Mikrostrukturphysik, DE-06120 Halle, Germany — [3]Max Planck Institute of Solid State Physics, DE-70569 Stuttgart, Germany — [4]Institute of Materials Chemistry, Vienna University of Technology, A-1060 Vienna, Austria — [5]CEA, DSM/IRAMIS/SPCSI/LENSIS, Bâtiment 462, F-91191, Gif-sur-Yvette cedex, France — [6]JARA Jülich-Aachen Research Alliance, Forschungszentrum Jülich, DE-52425 Jülich — [7]Fakultät für Physik and Center for Nanointegration Duisburg-Essen (CeNIDE), DE-47048 Duisburg, Germany

In $PbTiO_3$ / $La_{0.7}Sr_{0.3}MnO_3$ nanostructure arrays we confirmed a self-organizing pattern consisting of out-of plane 180° ferroelectric domains. The pattern was observed in Piezo-Force microscopy (PFM) as well as X-ray absorption spectroscopy (XAS) and threshold photoemission (TPES) using X-ray Photoemission Electron Microscopy (XPEEM). As found by PFM and XAS, the pattern correlates with the LSMO thickness as well as with the Mn valency state, indicating an electronic reconstruction at the interface. The observed effects could provide new ways of constructing multiferroic or magnetoelectric devices tuning the LSMO magnetism.

DF 19.6 Wed 15:00 Poster B2

Structural and Compositional Inhomogeneity of a Fe-SrTiO3 Film Studied by Electron Microscopy and Spectroscopy — •Hongchu Du[1,2,3], Chun-Lin Jia[1,2], and Joachim Mayer[1,2,3] — [1]Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany — [3]Gemeinschaftslabor für Elektronenmikroskopie (GFE), RWTH Aachen, Aachen, 52074, Germany

Lattice defects are essential for the microscopic switching mechanism in all the classes of the resistive switching effects. Hence a thorough understanding of electronically active defects is required to be able to correlate microscopic structures with the resistively switching properties.

Aberration corrected High-resolution (S)TEM provides real structural analysis down to the atomic level. Different techniques like HRTEM, ADF-STEM, and EELS enable revealing the microscopic details of the electronically active defects, thereby allowing a better understanding of how lattice defects interrelate with the resistively switching effects.

In this study, we observed that the Fe-SrTiO3 film has structural and compositional inhomogeneity by HRTEM, STEM, and EELS. Lattice parameter increment was observed in both the distort particle-like area and antiphase boundaries. The antiphase boundaries may be formed by 1/2 unit cell displacement of the antiphase domain in [110] direction with respect to the film. EELS profile shows that Fe are mainly distributed in the film. Enrichment of Fe was found in the strained area and at the interface.

DF 19.7 Wed 15:00 Poster B2

Kelvin probe force microscopy investigations of the contact charging of single crystalline insulators — •Monika Mirkowska[1,2], Markus Kratzer[2], Christian Teichert[2], and Helmut Flachberger[1] — [1]Chair of Mineral Processing, Department Mineral Resources and Petroleum Engineering, Montanuniversität Leoben, Austria — [2]Institute of Physics, Montanuniversität Leoben, Austria

Detailed knowledge about the contact charging behavior of dielectric materials is of great interest for technological applications like tribocharging separation of mineral particles. The underlying mechanisms are still not well understood. Here, an attempt is made to study the electric charging of well-defined surfaces (quartz and calcite monocrystals) upon contact with a conventional AFM tip. Measurements were performed in a fluid cell under controlled temperature (30 * 100 °C) and relative humidity (4 * 40 % RH) conditions. Kelvin probe force microscopy was applied to verify the electrostatic characteristic of the surfaces before and after contact charging. Both, tribocharging due to rubbing and static contact charging with applied tip bias have been investigated. The influence of humidity, contact time, contact force, and probe bias has been studied. The relative humidity turned out to play a key role in the charging process.

DF 19.8 Wed 15:00 Poster B2

Laser-induced nanostructure fabrication in fused silica surfaces: experiment and theory — •Pierre Lorenz, Frank Frost, Martin Ehrhardt, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

The fabrication of dielectric nanostructures is a big challenge for laser methods. The IPSM - LIFE method (IPSM - LIFE: laser induced front side etching using in situ pre-structured metal layers) allows the easy and fast production of complex surface structures into dielectric with lateral sizes down to 20 nm. At the IPSM - LIFE process, the irradiation of thin metal film deposited onto the fused silica substrate with low laser fluences results in the formation of complex metal structures by self-assembly processes and to a formation of a surface structure into the dielectric due to the melting, restructuring and resolidification of the dielectric surface. Further laser irradiation of the formed metal structures with high laser fluences causes the formation of complex patterns at the dielectric surface. The resultant structures were studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). The experimental results were compared with surface structures obtained from finite element method (FEM) simulations.

DF 19.9 Wed 15:00 Poster B2

Determination of the quality factor of microstructured dielectric surfaces by wave-front reconstruction — •Kay-Michael Voit, Hauke Bruening, Juliane Tschentscher, and Mirco Imlau — School of Physics, Osnabrueck University, Osnabrueck, Germany

We present our research results on the determination of the quality factor Q of micro- and nanostructured surfaces by means of (non-)linear light-matter interaction. Such structured surfaces play an important role in the field of advanced functional materials e.g. in nonlinear optics/photonics. However, there is so far no method for a contact-free, nondestructive control of the structure during synthesis and/or probing the structures' lifetime. First, an experimental setup for the optical measurement of periodic micro- and nanostructured surfaces within the range of $0 < Q < 1$ an $\delta Q = 0.1$ is presented. Taking into account the related boundary conditions, we show simulations of the optical far-field pattern resulting from microstructures with different quality factors. The wave front reconstruction is performed by a mixture of ray-tracing and Fresnel-Huygens/Kirchhoff diffraction theory. Possibilities for in-field application and calibration are discussed and a comparison between theoretical and experimental results is given.

DF 19.10 Wed 15:00 Poster B2

Electronic Structure of Rare-Earth Scandates $RScO_3$ (R= Pr, Nd, Sm, Eu, Gd, Tb, and Dy) — •Karsten Kuepper[1], Christine Derks[1], Andrei Postnikov[2], Reinhard Uecker[3], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]LCP-A2MC, University of Lorraine, F-57078 Metz, France — [3]Institute for Crystal Growth, D-12489 Berlin

Scandium based double oxides with other rare earth lanthanides of type $RScO_3$ (R=Pr,Nd,Sm,Eu,Gd,Tb, and Dy) find a number of potential interesting applications, first of all in its quality of a high dielectric constant (high-k) material. Here we present the results of a detailed electronic structure investigation, applying a number of complementary x-ray spectroscopic techniques, namely x-ray photoelectron spectroscopy (XPS), x-ray absorption spectroscopy (XAS), and x-ray emission spectroscopy (XES) in combination with theoretical LDA+U electronic structure calculations [1,2,3]. We find an overall excellent agreement between experiment and theory. Furthermore, we discuss a band gap variation in dependence of R, analyzed by means of O K XAS and XES [2].

[1] M. Raekers et al., Phys. Rev. B 79, 125114 (2009).
[2] C. Derks et al., Phys. Rev. B 86, 155124 (2012).
[3] A.V. Postnikov et al., Ferrolelectrics, in press.

DF 19.11 Wed 15:00 Poster B2

Oxygen Related Defects and the Reliability of Strained High-κ Dielectric Films in Field Effect Transistors: A First Principles Investigation — •Ebrahim Nadimi[1,2,4], Rolf Öttking[2], Philipp Plänitz[2], Martin Trentzsch[3], Christian Radehaus[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz — [2]GWT-TUD GmbH Geschäftsstelle Chemnitz — [3]Global Foundries, D-01109 Dresden, Germany — [4]Faculty of Electrical and Computer Engineering, K.N. Toosi University of Technology, Tehran, Iran

The strain engineering of the silicon channel in metal-oxide-field-effect transistors (MOSFET) along with the high-k (HK) and metal gate (MG) technology has been used in order to improve the performance of these transistors. Applying both techniques raises the question: what would be the interaction of these two techniques. The main concern in HK/MG stacks is the reliability and degradation of the gate dielectric which is mainly related to the oxygen vacancies. In this work we try to study the influence of mechanical stress on the electronic properties of such defects. First principles calculations based on the density functional theory and beyond that (hybrid functionals) were applied to investigate the formation energy and induced trap levels. The calculations reveal that mainly the charged defects are responding to the mechanical stress. In agreement with experimental results which show larger negative bias temperature instability (NBTI) for compressively stressed samples, the calculated formation energy of positively charged defects reduces by compressive stress while it rises with tensile stress.

DF 19.12 Wed 15:00 Poster B2

Restoring the k-value in damaged ultra-low k materials — •Oliver Böhm[1,2], Roman Leitsmann[2], Philipp Plänitz[2], Thomas Oszinda[3], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]AQcomputare GmbH, Annaberger Str. 240, 09125 Chemnitz, Germany — [3]GLOBALFOUNDRIES Dresden Module Two GmbH & Co. KG, Germany

The decreasing feature size of integrated circuits results in a smaller distance between the conduction layers, which is accompanied by an increasing resistance capacitance (RC) delay. To reduce this effect materials with an ultra-low dielectric constant can be used. However, the technical application of ultra-low k (ULK) materials is connected to several problems. After the etching of trenches or vias typically a considerable amount of carbon depletion and subsequently the formation of OH-groups can be observed. This results in moisture uptake and consequently in a strongly increased dielectric constant. To restore the k-value, a post-etch treatment is necessary.

In this study we use state of the art density functional theory (DFT) combined with a nudged elastic band (NEB) method to investigate different silylation processes. The efficiency of several silazanes and siloxanes will be compared. Furthermore, the influence of other post-etch treatments on the k-restoring will be briefly discussed. Finally, based on the obtained results an improved scheme for the k-restoring

process of ultra-low k materials will be proposed.

DF 19.13 Wed 15:00 Poster B2

Microgoblet Lasers for Label-free Biosensing — •Jan Fischer[1], Sarah Wiegele[1], Tobias Grossmann[1], Torsten Beck[1], Martin Mai[1], Uwe Bog[2], Timo Mappes[2], and Heinz Kalt[1] — [1]Institut für Angewandte Physik, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institut für Mikrostrukturtechnik, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Biosensors for label-free detection offer a huge variety of applications in life science. We report on laser dyes embedded in goblet-shaped polymeric microresonators. These resonators are fabricated in a simple and low-cost manufacturing process suitable for mass production. The dye-doped polymer poly(methyl methacrylate) (PMMA) is directly processed on a silicon substrate. The developing and etching process is followed by a thermal reflow step which smoothes the surface and enhances the Q-factor significantly. The emission of these microgoblet lasers is in the visible region and can be varied using different laser dyes. The surface of the resonators can be functionalized with different receptors sensitive to wanted molecules. Binding of molecules can be detected by measuring the spectral shift of the resonant whispering gallery mode.

DF 19.14 Wed 15:00 Poster B2

Ultrafast holographic spectroscopy — •Andreas Buescher, Kay-Michael Voit, Hauke Bruening, Holger Badorreck, and Mirco Imlau — School of Physics, Osnabrueck University, Germany

A novel experimental approach for the study of small-polaron-related changes of the complex permittivity in lithium niobate is presented. Our approach is based on holographic spectroscopy [K. Voit and M. Imlau, Materials (2013)] that has been established as an important tool for the analysis of light-induced changes of the complex dielectric permittivity at optical frequencies. The study of dispersive permittivity features in lithium niobate is driven by our recent discovery of efficient small-polaron based hologram recording with single laser pulses [H. Bruening et al., Opt. Express **20**, 13326 (2012)]. In order to study the underlying mechanisms, holographic spectroscopy must be extended to a dynamic tool with temporal resolution of the small polaron formation time ($\approx 100\,fs$). We have addressed this demand by the design of a novel type of nonlinear optical setup that includes holographic techniques, a broad-band probing light source by means of supercontinuum generation as well as a classical pump-probe setup equipped with an optical delay line for sub-ps temporal resolution. The concept is verified experimentally using Fe-doped lithium niobate.
Financial support by the Deutsche Forschungsgemeinschaft (IM 37/5, INST190/137-1) is gratefully acknowledged.

DF 19.15 Wed 15:00 Poster B2

Simulation of the melting temperature reduction of TiO_2 by oxygen deficiency — •Jason Marx, Jan Michael Knaup, and Thomas Frauenheim — BCCMS, Universität Bremen, Germany

The memristive effect in TiO_2 is governed by the externally driven migration of oxygen in a reduced bulk oxide. In the unipolar switching regime, this defect migration leads to the formation and dissolution of metallic Ti_4O_7 nanofilaments through the insulating bulk TiO_{2-x}. The mechanism of this phase transition is so far not understood at all. One possibility is the local melting of the bulk titania which is usually either amorphous or in the rutile structure followed crystallization into the Ti_4O_7 Magnéli phase upon cooling. As an initial step towards understanding the formation of Magnéli phase nanofilaments, we perform Density-Functional based Tight-Binding (DFTB) modeluclar dynamics (MD) simulations of bulk TiO_{2-x} at defect concentrations ranging from 0 to the equivalent of Ti_4O_7 stoichiometry at constant cell volume. From the particle trajectories we deduce the melting point by analyzing the RDF, the self-diffusion coefficient and the Linemann index. Special care is taken to analyze the actual dynamics properties of the material, instead of thermostat artifacts. We find a significant lowering of the the melting temperature with rising defect concentration. This lowering is larger than can be explained by the reduction in excluded volume alone. The results indicate that local variations in defect concentration leading to local melting point variations play an important role in the filament formation process.

DF 19.16 Wed 15:00 Poster B2

Piezoresponse force microscopy studies of (K,Na)NbO3-based ceramics for piezoactuator applications — •Danka Gobeljic[1], Vladimir V. Shvartsman[1], Ke Wang[2], Wook Jo[3], Jing-Feng Li[2], Jürgen Rödel[3], and Doru C. Lupascu[1] — [1]Institute for Materials Science, Universität Duisburg-Essen, Essen 45141, Germany — [2]State Key Laboratory of New Ceramics and Fine Processing, Tsinghua University, Beijing 10008, P.R. China — [3]Institute of Materials Science, Technische Universität Darmstadt, Darmstadt 64287, Germany

One of the most promising, environmentally friendly, lead-free piezoceramics are (K,Na)NbO3 (KNN)-based materials. Purposeful doping makes KNN especially suitable for high-precision, temperature-stable actuator applications, providing high piezoelectric constant d33 and strain, which shows significant stability in a range from room temperature up to 175°C. We present results of a Piezoresponse Force Microscopy (PFM) study on 0.95(Na0.49K0.49Li0.02)(Nb0.8Ta0.2)O3-0.05CaZrO3 ceramics at different temperatures. For both poled and unpoled states of KNN samples a reorganization of domain structure was observed with temperature increase. It is related to a sequence of phase transformation in this material. Measured temperature dependences of the local longitudinal piezoelectric coefficients are in reasonable agreement with temperature behavior of the macroscopic low signal piezoelectric coefficient. Obtained results provide nanoscopic insight on mechanisms of enhanced electromechanical properties in the studied KNN-based ceramics.

DF 19.17 Wed 15:00 Poster B2

Electrical and optical properties of tungsten doped VO_2 thin films — •Sebastian Vatterodt[1], Jura Rensberg[1], Danilo Buerger[2], Heidemarie Schmidt[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [2]Institut für Materialsysteme der Nanoelektronik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Single crystalline vanadium oxide (VO_2) undergoes a reversible metal to insulator transition (MIT) accompanied by a structural transition from metallic rutile phase (R) to insulating monoclinic phase (M1) at a temperature of about 68°C. Most likely, this transition is caused by electron-electron correlation which leads to a splitting of the V^{4+} 3d valence band. Therefore, a band gap with an energy of about 0.6 eV is observed in the insulating phase. Furthermore, it is well known that the transition temperature in VO_2 can be decreased by high valent dopants, i.e. tungsten, which are incorporated into the lattice. Here we investigated the influence of tungsten doping on the electronic structure. Thus we grew VO_2 thin films on sapphire by pulsed laser deposition (PLD) with different tungsten content. The films were characterized by measuring both their transmittance in the UV-VIS-NIR spectral range and their sheet resistivity as a function of the temperature. The changes of the electronic structure, i.e. the position of the V^{4+} 3d band, due to tungsten doping are discussed and compared with theoretical band structure calculations.

DF 19.18 Wed 15:00 Poster B2

Nanoscale characterization of electroactive polymer nanocomposites with ferroelectric crystalline additions — Dmitry Kiselev[1], •Vladimir Shvartsman[2], Maksim Silibin[3], Alexander Solnyshkin[3], and Doru Lupascu[2] — [1]National University of Science and Technology (MISiS), Moscow, Russia — [2]Institut für Materialwissenschaft, Universität Duisburg-Essen, Essen, Germany — [3]National Research University of Electronic Technology (MIET), Moscow, Russia

Ferroelectric polymers, in particular polyvinylidene fluoride (PVDF) and its copolymers, offer an attractive combination of properties such as relatively high spontaneous polarization, piezoelectricity, chemically inert behavior, electrical strength, and durability. Recently, attention of researchers has more and more often been attracted to objects simultaneously having properties of polymers and classical ferroelectrics. Such objects are composite films based on polymeric materials with addition of ferroelectrics, e. g. barium lead zirconate titanate (BPZT).

In this work, we report on local ferroelectric and piezoelectric properties of nanostructured polymer composites P(VDF-TrFE)+xBPZT (x = 0 - 50 %). High-resolution imaging of ferroelectric domains, local polarization switching, and polarization relaxation dynamics were studied by piezoresponse force microscopy. In particular, we found that BPZT inclusion usually show a strong unipolar piezoresponse signal, as compared to the polymer matrix. By scanning under high dc voltage films can be polarized uniformly under both positive and negative electric fields. Stabilty of the polarized state is discussed.

DF 19.19 Wed 15:00 Poster B2

Measurement of Elastic Properties of Some Epoxy Materials in a Broad Frequency Range — •Ulrich Straube[1], Christoph Pientschke[1,2], and Sabine Kern[1,2] — [1]Martin-Luther-University Halle, Institute of Physics, Germany — [2]Martin-Luther-University Halle, Interdisciplinary Center of Materials Science, Germany

Composite materials containing embedded piezoelectric fibers in epoxy materials are important for the fabrication of ultrasound transducers for medical applications. The elastic stiffness and compliance coefficients of these epoxy materials must be known for optimising and modeling of such composites.

Measurement methods for the determination of the Young's modulus and the shear elastic modulus are described. The methods contain the Hz-range with dynamical mechanical analysis (DMA), mechanical resonator methods in the kHz-range and several ultrasound methods in the lower MHz-range.

These methods are utilized for the mechanical characterisation of epoxy materials used in ultrasound transducers. Selected results spanning a broad frequency range are presented.

DF 19.20 Wed 15:00 Poster B2

Large-scale 3D simulation and analysis of acoustic waves in piezoelectric materials — •Tristan Koppe, Julian Amani, Hans Hofsäss, and Ulrich Vetter — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Bulk and surface acoustic waves (BAW/SAW) are used to create compact, cost-efficient and easy to produce (sometimes even CMOS compatible) high frequency filters, resonators and compressors with superior properties essential for modern mobile and wireless communications. Numerical simulations of SAW/BAW structures have become a powerful tool for research and development of new devices and applications. A finite element package for SAW and BAW simulations has been designed to describe non-periodic three dimensional SAW/BAW devices in time domain. The simulation features the computation of systems with several million elements. Especially 2H-AlN thin films on substrates with various interdigital transducer configurations are considered.

DF 19.21 Wed 15:00 Poster B2

Time-domain large-signal simulation of electrical equivalent circuits with non-linear components — •Julian Alexander Amani, Tristan Koppe, Hans Hofsäss, and Ulrich Vetter — II. Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland

When investigating dielectric properties of a heterostructure, simulation of electrical equivalent circuits (EECs), modelling the measured impedance response, has proven useful to identify different contributions to the system.

An in-house developed simulation software capable of including arbitrary, even non-linear, resistance or capacitance models is presented. It utilises bias voltage, signal amplitude, frequency and temperature dependence of each element to calculate the impedance response of the circuit. Considering signal amplitude facilitates simulation of non-linear responses, in addition to the linear response of the system. Time-domain analysis permits extraction of the calculated signal over time at each component, thus allowing hypothetical oscilloscope measurements at each, even usually experimentally inaccessible, component.

Variation of additional parameters (e. g. bias voltage, temperature) allows eliminating circuit ambiguity. However, usually the measured frequency response is fitted without varying another parameter or for each variation separately. Since this software considers the response of each element to the varying parameter, the comparison of measured and calculated results is done in the full parameter space instead of fitting single frequency responses.

DF 19.22 Wed 15:00 Poster B2

Characterisation of nonlinear capacitors as alternative energy storage — •Sebastian Lemm[1], Wolfram Münchgesang[1], Martin Diestelhorst[1], Mandy Zenkner[2], Thomas Grossmann[2], Claudia Ehrhardt[2], Jens Glenneberg[3], Alexandra Buchsteiner[3], Horst Beige[1], Stefan G. Ebbinghaus[2], and Hartmut S. Leipner[3] — [1]Institute of Physics, Martin-Luther-University, D-06099 Halle, Germany — [2]Institute of Chemistry, Martin-Luther-University, D-06099 Halle, Germany — [3]Interdisciplinary Center of Materials Science , Martin-Luther-University, D-06099 Halle, Germany

The storage of energy requires the knowledge of the DC properties of the dielectric inside the capacitor. To characterise eligible materials like $BaTiO_3$ for this special application we performed measurements under AC and DC conditions. As could be shown AC measurements are only of limited suitability to draw conclusions about the applicability of the materials. In the presentation we compare different measerement methods like DC charge-discharge measurements, low frequency measurements of the dielectric permittivity, and DC-conductivity which were performed on samples of different compositions like thin films of spin coated $BaTiO_3$-polymer composites and $BaTiO_3$-composites with anorganic matrix. Furthermore we tried to find correlations between the macroscopic dielectric properties and the microstructure of the materials investigating the materials by ESEM and TEM. It has been proven that a complicated interplay between many microscopic effects is responsible for the macroscopic dielectric properties.

The work was supported by BMBF within the project Superkon.

DF 19.23 Wed 15:00 Poster B2

Holographic image recording in nominally undoped, thermally reduced $LiNbO_3$ using small bound polarons — •Sarah Masch, Hauke Brüning, and Mirco Imlau — School of Physics, Osnabrück University, Germany

An experimental setup for the study of holographic image recording is presented that uses a new type of hologram recording mechanism in nominally undoped, thermally reduced $LiNbO_3$. By means of single intense ns-laser pulses ($\lambda = 532\,\mathrm{nm}$) short-lived volume gratings with high diffraction efficiencies occur [1,2]. These gratings are based on spatially modulated densities of small bound polarons and can be described as mixed gratings as they originate from both the light-induced absorption of the polarons as well as from a polaronic change of the refractive index. Due to their fast generation on the fs-scale, such small polaron-based gratings offer unique properties needed for real-time holographic applications. We demonstrate the successful application of this type of recording mechanism using cross polarized beams for both recording and read-out. The impact of our findings for ultrafast real-time holography is discussed.

[1] H. Bruening et al., Optics Express 20, 13326 (2012)

[2] M. Imlau et al., Optics Express 19, 15322 (2011)

*Financial support by the DFG (IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.