# DF 15: Thin Films and Nanostructures II

Time: Thursday 10:40–13:00 Location: WIL B321

DF 15.1 Thu 10:40 WIL B321

**Interface effects in solid electrolytes** — •Björn Martin and Herbert Kliem — Saarland University, Germany

To investigate interface effects, thin films of ion conducting polyethylene oxide (PEO) doped with different salt concentrations are used. Capacitance structures with evaporated Al or Cu electrodes are assembled. An ionic space charge polarization prevails in these systems.

For computer simulations, a three-dimensional discrete hopping model is developed. Negative ions can fluctuate thermally activated over energy barriers in a multiwell potential. The interactions of the ions with the electrodes are considered using the method of images. Also, electrostatic interactions between all ions and between the ions and a positive background charge providing neutrality are considered.

The attractive Coulomb forces between the original charges and the image charges cause a charge accumulation at the electrodes even without applied field as predicted in the simulations. Due to the repulsive forces of these accumulation layers a depletion of mobile charges towards the volume of the sample is found. This charge distribution causes an internal potential with a maximum in the middle of the sample. In the experiment, this potential distribution can be determined using a scanning Kelvin probe which detects the surface potential between the electrodes.

Furthermore, the electrode effects are responsible for the dynamic behavior of the systems like the Kohlrausch behavior of the polarization current and thus the increase of the dielectric permittivity at low frequencies, and the onset of charge injection.

DF 15.2 Thu 11:00 WIL B321

**Characterization of $PbSc_{0.5}Ta_{0.5}O_3$ epitaxial thin films prepared by Pulsed Laser Deposition** — •Anuj Chopra, Marin Alexe, Balaji Ishwarrao Birajdar, Ionela Vrejoiu, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Halle, D-06120, Germany

Epitaxial $PbSc_{0.5}Ta_{0.5}O_3$ (100) (PST) thin films of thickness 70 nm were deposited on vicinal $SrTiO_3$ (STO) (100) substrates with a layer of $SrRuO_3$ (SRO) as a bottom electrode by pulsed laser deposition (PLD) at 823K. Their crystal orientation, topography and microstructure were analysed by X-ray diffraction, atomic force microscopy (AFM) and transmission electron microscopy (TEM), respectively. The films deposited at temperature higher than 823K showed the presence of pyrochlore phase whereas films grown at 823K were perovskites. The in-plane and out-of-plane epitaxial relationships were studied by $\Phi$ and $\theta$-$2\theta$ scans respectively. AFM revealed a smooth surface with RMS of 1.1nm. Superstructure reflections obtained in the TEM diffraction patterns of the films confirm cation ordering. The films were characterized by using polarization vs electric field (P-E) and switching current vs voltage (I-V) measurements. Polarization of the epitaxial films at zero electric field was $2\mu C/cm^2$ at room temperature. Cation ordering with post annealing of the films is still under investigation. This work describes the preparation and characterization of epitaxial films of PST (100) for the first time and indicates PST as a potential candidate for infra-red image sensor applications.

DF 15.3 Thu 11:20 WIL B321

**Switching kinetics in epitaxial $BiFeO_3$ thin films with different orientations** — •Daniel Pantel[1], Ying-Hao Chu[2], Ramamoorthy Ramesh[3], and Marin Alexe[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — [2]Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan 30010, R.O.C. — [3]Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

Due to simultaneously ferroelectric and antiferromagnetic ordering at room temperature multiferroic $BiFeO_3$ (BFO) is a potential material for magnetoelectric devices. Furthermore, it is a Pb-free ferroelectric with high remnant polarization and therefore a promising candidate for environmental-friendly applications such as non-volatile memories. For all applications understanding of the detailed switching behavior in BFO is essential.

Large timescale (100 ns to 1 s) voltage pulse trains were used to examine the switching kinetics in BFO thin films with (001), (110) and (111) orientations as a function of applied voltage and time. The kinetics are analyzed in terms of Kolmogorov-Avrami-Ishibashi (KAI) theory and compared with standard systems such as epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ (PZT) films. Likewise in fully c-oriented PZT films, BFO fits well the KAI-model in the high field region, whereas the low field region shows non-KAI kinetics comparable with PZT films with 90 ° domain walls.

DF 15.4 Thu 11:40 WIL B321

**Stabilization of out-of-plane polarization and head-to-head 180° domain walls in ferroelectric materials** — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Experimental studies suggest that defects play an important role in ferroelectric materials. Employing density functional theory calculations based on the full-potential linearized augmented planewave method as implemented in the FLEUR code (www.flapw.de), we studied the polarization perpendicular to the surface of thin films of the ferroelectric perovskites $BaTiO_3$ and $PbTiO_3$. Without an electric field that compensates the depolarization field a polarization perpendicular to the surface is not stable, but we can stabilize an out-of-plane polarization with different types of defects at the surface. This mechanism can also be at work at head-to-head and tail-to-tail 180° domain walls, which can occur in these compounds. Although nominally a substantial extra charge is present at these surfaces or interfaces, the electronic properties are found to be very similar to the bulk of the perovskites.

DF 15.5 Thu 12:00 WIL B321

**Study of polyimide after graphitization with low-energy $Ar^+$ Ion irradiation by NEXAFS** — •Marcel Michling[1], Daniel Friedrich[1], Dieter Schmeisser[1], Yuri Koval[2], and Paul Müller[2] — [1]Brandenburgisch Technische Universität Cottbus, Angewandte Physik/Sensorik, K.- Wachsmann-Allee 1, 03046 Cottbus — [2]Universität Erlangen Nürnberg, Experimental Physik/Supraleitung, Erwin-Rommel-Str. 1, 91058 Erlangen

In this contribution we report on investigations of the electronic structure of $Ar^+$ irradiated polyimide samples by using NEXAFS. The NEXAFS measurements were done at the U49/2-PGM2 beam line of BESSY II, Berlin using TEY and TFY detection.
Polyimide samples are prepared using low $Ar^+$ dose while the temperature of the samples is varied between 300K and 700K. In the NEXAFS data at the Carbon K-edge we see substantial changes between different samples. The differences appear in particular in the more surface sensitive TEY-Signal.
The NEXFS data are consistent with the graphitization of the surface upon $Ar^+$ bombardment as we identify the characteristic absorption bands of graphitic carbon. Its relative content increases with increasing sample temperature. In contrast, in the more bulk sensitive TFY data, the emission characteristic of polyimide is maintained.
The possibility to cover insulating polymers with a conducting layer is a great demand for many applications. Because of the relative low price of the basic materials, the irradiation with low-energy Ions will play an important roll in the microelectronic of the future.

DF 15.6 Thu 12:20 WIL B321

**Effects of rare earth manganite on structural, magnetic and ferroelectric properties of $BiFeO_3$ thin films** — •Abdelilah Lahmar, Salah Habouti, Matthias Dietze, Claus-Henning Solterbeck, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

The results of structural studies of pure-phase perovskite thin films of $BiFeO_3$ – 10% $RMnO_3$ (R= La, Eu, Gd, Tb and Dy) are presented. Raman Scattering studies show lines broadening similar to what is reported for $RMnO_3$; they were attributed to Jahn-Teller distortion and orthorhombic structural change. Evidence of an anomaly of the orthorhombic distortion at $GdMnO_3$ could be obtained. Interestingly the addition of $GdMnO_3$ leads to a substantial increase in magnetization, combined with moderate ferroelectric polarization. All other compositions are characterized by higher ferroelectric polarization but almost no magnetization.

DF 15.7 Thu 12:40 WIL B321

**Growth of Conductive $HfO_{2-x}$ Thin Films by Reactive Molecular Beam Epitaxy** — •Erwin Hildebrandt[1], Jose Kurian[1], Hans-Joachim Kleebe[2], and Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU Darmstadt, Germany — [2]Institut für Angewandte Geowissenschaften, TU Darmstadt, Germany

Thin films of oxygen deficient hafnium oxide were grown on single crystal $c$-cut and $r$-cut sapphire substrates by reactive molecular beam epitaxy. The oxidation conditions during growth were varied within a wide range using RF-activated oxygen. Hafnium oxide thin films were characterized using X-ray diffraction, resistivity measurements ($\rho$-T) and transmission electron microscopy (TEM). The results show a dramatic increase in conductivity of the deposited oxygen deficient hafnium oxide thin films with decreasing oxidation conditions during growth. The electrical properties of deficient hafnium oxide thin films varied from insulating over semiconducting to conducting. X-ray diffraction data as well as TEM data rule out the possibility of conductivity due to metallic hafnium.