DF 8: Electrical and mechanical properties

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

DF 8.1 Tue 14:00 H9

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

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

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

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

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

DF 8.2 Tue 14:20 H9

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

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

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

DF 8.3 Tue 14:40 H9

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

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

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

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

DF 8.4 Tue 15:00 H9

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

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

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

DF 8.5 Tue 15:20 H9

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

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

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

DF 8.6 Tue 15:40 H9

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

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

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

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