KR 3: Electrical and mechanical properties (DF jointly with KR)

Time: Monday 15:00–16:00 Location: H11

KR 3.1 Mon 15:00 H11

High-pressure crystal structure of $Bi_{12}GeO_{20}$ sillenite — •Leonore Wiehl, Alexandra Friedrich, Eiken Haussühl, Wolfgang Morgenroth, and Björn Winkler — Institut für Geowissenschaften, Goethe-Universität, Frankfurt/Main, Germany

$Bi_{12}GeO_{20}$ crystallizes in the sillenites structure type with the noncentrosymmetric cubic space group $I23$. Sillenites $Bi_{12}MO_{20}$ (M = Si, Ge, Ti) are used in technical applications because of their outstanding electrical and nonlinear optical properties, especially the photorefractive effect. These properties are assumed to be correlated with the stereochemical activity of the $6s^2$ lone electron pair of Bi^{3+}.

The evolution of the $Bi_{12}GeO_{20}$ crystal structure under high pressure was investigated by experiment and theory using single-crystal X-ray diffraction and density functional theory (DFT) calculations. The crystal structure was determined from X-ray intensity data collected at ambient conditions in house and at high pressure with synchrotron radiation at HASYLAB (D3). Pressures up to 21 GPa were generated in diamond anvil cells. DFT calculations were performed up to 50 GPa. The pressure dependence of interatomic distances indicates a reduced eccentricity of the Bi^{3+} coordination at high pressure, but not a collapse of the Bi^{3+} lone electron pair. The results are discussed in comparison with the isotypic Si sillenite [1].

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[1] Wiehl L, et al. (2010) J. Phys.: Condens. Matter 22, 505401

KR 3.2 Mon 15:20 H11

Ripening of ZnO nanoparticles - influence of the stabilizing layer — •Torben Schindler, Martin Schmiele, Thaer Kassar, and Tobias Unruh — Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander Universität Erlangen Nürnberg, Staudtstr. 3, 91058 Erlangen

ZnO semiconductor nanoparticles (NPs) exhibit promising electro-optical properties for applications in e.g. solar cells or light emitting devices due to the quantum size effect. Thus, the preparation of well-defined, stable ZnO-NPs is of high interest and therefore knowledge about the nucleation and growth processes is crucial.

For the synthesis ethanolic solutions of zincacetate and lithiumhydroxide are simply mixed. The nucleation of the NP occurs instantly, while a further ripening of the ZnO-NPs starting from about 2.5 nm as a function of temperature was observed using UV/Vis measurements. The ripening process is further investigated in detail using temperature- and time-dependent small angle x ray scattering (SAXS) measurements. To determine the influence of the stabilizing acetate layer for the particle growth, small angle neutron scattering (SANS) is used and first results will be presented.

KR 3.3 Mon 15:40 H11

Localization Effects in Dielectric Disordered Crystals and Random Materials — Anton Lebedev, Marius Dommermuth, and •Regine Frank — Institut für Theoretsiche Physik, Universität Tübingen

Anderson localization, the counterpart of hyper diffusion, more than ever is of high interest to the semiconductor community. We apply diagrammatic quantum field theory beyond Lippmann-Schwinger equation to derive and explain localization effects in disordered photonic crystals and random media. Mie-Scattering als well as other scatterers are considered and we present self-consistent fit-parameter free 'ab initio' calculations and results.