DF 8 Spectroscopy, Scanning and Diffraction Methods

Time: Wednesday 14:30–16:50 Room: MÜL Elch

Invited Talk DF 8.1 Wed 14:30 MÜL Elch

Phonons in multiferroics: BiFeO3 and related systems — •Jens Kreisel[1], Raphaël Haumont[1,2], Pierre Bouvier[3], and Françoise Hippert[1] — [1]ENS de Physique de Grenoble (F), CNRS — [2]Université d'Orsay (F) — [3]ENSEE Grenoble (F), CNRS

On the way towards a fundamental understanding of magnetoelectric multiferroics the experimental observation and understanding of the coupling mechanism between the ferroelectric and magnetic order are of great interest. Very little is currently known about the behavior of phonons in magnetoelectric multiferroics, and this although investigations of phonons have in the past played a crucial role in the understanding of classic ferroelectrics.

Motivated to determine and understand the role of phonons in multiferroics, we will discuss the phonon spectrum measured by Raman spectroscopy of the model system bismuth ferrite BiFeO3 (BFO). Further to the discussion of Raman spectra from BFO powder, single crystalline and thin film samples we will compare our results to those from similar but not multiferroic RFeO3 samples.

Key points that will be addressed are: 1) A paraelectric-to-ferroelectric phase transition which is not soft-mode-driven in BFO, 2) Colossal phonon anomalies for BFO around the Néel temperature for some particular phonons, while this is not observed for non multiferroic EuFeO3. The results are discussed in the context of spin-phonon coupling and interactions between magnetic and ferroelectric order parameters. 3) A significant difference in Raman spectra between bulk and thin film BFO samples illustrating the role of epitaxial strain.

DF 8.2 Wed 15:10 MÜL Elch

Luminescent spectroscopy of the RE ions incorporated in the lead tungstate crystals — •Oksana Chukova[1], Sergiy Nedilko[1], and Marian Pashkovskyi[2] — [1]Physics Faculty, Kyiv National Taras Shevchenko University 2, block 1, acad. Hlushkov Ave., 03680, Kyiv, Ukraine — [2]Physics Faculty, Lviv National Ivan Franko University, Lviv, Ukraine

The lead tungstate $PbWO_4$ (PWO) crystals are widely doped by various impurities, especially rare earth (RE) ions, in order to change characteristics of these crystals, e.g., significantly improve transmission and radiation hardness of the crystal. Spectral properties of the RE doped PWO crystals were studied formerly, but the investigations were directed mainly on spectroscopy of proper matrix emission of the pure and doped crystals. The present paper is concentrated on investigation of spectroscopy of RE ions in the PWO crystal matrix. Spectral properties of the Pr^{3+} and Eu^{3+} ions doped into the PWO crystal were studied at photo and synchrotron radiation excitation and analyzed on parameters of Stark splitting in the crystal field. Formation of at least two types of emission centers based on the RE ions in the PWO crystal lattice is shown and origin, structure and spectroscopy of these centers are investigated. Different site symmetry and oxygen coordination influence in different ways on probabilities of emission and excitation transitions as well as on shifts of lines and weight centers of manifolds for the both types of centers. Experiments with synchrotron excitation were performed at SUPERLUMI Station at HASYLAB, DESY, Hamburg.

DF 8.3 Wed 15:30 MÜL Elch

Rare-earth doped barium halide x-ray storage phosphors and scintillators — •Julia Selling and Stefan Schweizer — Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Rare-earth (RE) doped orthorhombic BaX_2 (X = Cl, Br, I) single crystals were investigated for their properties as x-ray storage phosphors and as x-ray scintillators by means of photoluminescence (PL), photostimulated luminescence (PSL) and x-ray luminescence (XL). The investigation of the storage and read-out mechanism in these materials will help to optimise the PSL effect in Eu- or Ce-doped fluorozirconate-based glass ceramics containing PSL-active BaX_2 nanoparticles which are formed upon thermal processing of the glass [1, 2]. The PSL efficiency of the single crystals is comparable to that of Eu-doped BaFBr, which is used in commercial x-ray storage phosphor screens. The scintillation efficiency of the RE-doped barium halides investigated is compared to that of CWO ($CdWO_4$). Features like afterglow or radiation hardness have not been considered in our comparison. The influence of the anion-cation distance on the intensity ratio of the emission types is discussed.

[1] A. Edgar, J.-M. Spaeth, S. Schweizer, S. Assmann, P.J. Newman, and D.R. Macfarlane, Appl. Phys. Lett. **75** (1999) 2386.

[2] S. Schweizer, L.W. Hobbs, M. Secu, J.-M. Spaeth, A. Edgar, G.V.M. Williams, Appl. Phys. Lett. **83** (2003) 449.

DF 8.4 Wed 15:50 MÜL Elch

Luminescent oxygen-vacancy complex in Mn-doped $LiBaF_3$ investigated by optically detected magnetic resonance — •Bastian Henke[1], Uldis Rogulis[2], and Stefan Schweizer[1] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Institute of Solid State Physics, University of Latvia, Riga, Latvia

Upon ultraviolet photoexcitation, Mn-doped $LiBaF_3$ shows different luminescence bands in the visible range. The luminescence, which can be attributed to Mn^{2+}, is at 712 nm [1], whereas two additional bands appear at 423 and 480 nm. The peaks at 423 and 480 nm have completely different excitation spectra than the one for the 712 nm emission, which shows the typical Mn^{2+} excitation bands. Photoluminescence detected electron paramagnetic resonance measurements yielded that the bands at 423 and 480 nm can be attributed to an oxygen-vacancy complex. Its principal axis, z, of the fine structure tensor is aligned along a <110> direction. The Mn^{2+}-dopant can be found in the vicinity of this complex. We assume that Mn^{2+} substitutes for a Ba^{2+} ion.

[1] B. Henke, M. Secu, U. Rogulis, S. Schweizer, J.-M. Spaeth, phys. stat. sol. (c) **2**, No. 1 (2005), 380

DF 8.5 Wed 16:10 MÜL Elch

Density-functional simulations for X-ray and Electron Holographic measurements of single crystal properties of tetragonal Bariumtitanate — •Axel Rother[1], Igor Chaplygin[2], Sibylle Gemming[2], Tillman Leisegang[1], Dirk Meyer[1], and Hannes Lichte[1] — [1]Institute of Structure Physics, Dresden University, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University, Germany

As a typical member of Ferroelectrics, tetragonal BaTiO3 reveals a lot of interesting properties such as the electric polarization along the tetragonal axis. Modern X-ray and Electron Holographic methods are able to measure these features by utilizing refinement with given theoretical models. Firstly, a single crystal X-ray reflection measurement was performed to obtain structural parameters and the electron density. Secondly, high resolution electron holography was utilized to measure the dipole character of the electric potential, and thirdly, different Density-functional simulations were carried out for a detailed comparison with the measured data. Furthermore we began to incorporate the theoretical calculations in the refinement models used in High Resolution Electron Holography.

[1] Support from DFG in the Framework of FOR 520 is gratefully acknowledged

DF 8.6 Wed 16:30 MÜL Elch

Density-functional simulations for X-ray and Electron Holographic measurements of single crystal properties of tetragonal Bariumtitanate — •Axel Rother[1], Igor Chaplygin[2], Sibylle Gemming[2], Tilmann Leisegang[1], Dirk Meyer[1], and Hannes Lichte[1] — [1]Institute of Structure Physics, Dresden University, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University, Dresden, Germany

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