TT 31: Matter at Low Temperature: Materials

Time: Wednesday 15:45–17:00 Location: HSZ 304

TT 31.1 Wed 15:45 HSZ 304

Modelling of the loss mechanisms in crystalline solids at low temperatures for future gravitational wave detectors — •Daniel Heinert[1], Alexander Grib[2], Christian Schwarz[1], Stefanie Kroker[1], Ronny Nawrodt[3], Wolfgang Vodel[1], Andreas Tünnermann[4], Sheila Rowan[3], Jim Hough[3], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Kharkov National University, Physics Department, 61077 Kharkov, Ukraine — [3]University of Glasgow, Institute for Gravitational Research, Kelvinbuilding, University Avenue, G12 8QQ Glasgow, Scotland — [4]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Mechanical losses play a crucial role in reducing thermal noise of future gravitational wave detectors. Low loss materials are needed at low temperatures to reduce thermal noise significantly.

We present a study of internal loss mechanisms in crystalline solids to understand the origin of dissipation. Exemplarily, the different loss contributions are described in crystalline quartz. The focus lies on thermoelastic losses and a contribution arising from the interaction of phonons. Then these results are applied to silicon as the most interesting material for the third generation of gravitational wave detectors.

This work is supported by the German science foundation DFG under contract SFB TR7.

TT 31.2 Wed 16:00 HSZ 304

Analysis of the electric field gradient in the perovskites $SrTiO_3$ and $BaTiO_3$: density functional and model calculations — •Katrin Koch[1], Roman Kuzian[2], Klaus Koepernik[3], and Helge Rosner[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden — [2]Institute for Problems of Materials Science, Kiev — [3]Leibniz Institute for Solid State and Materials Research, Dresden

We analyze recent measurements [1] of the electric field gradient on the oxygen site in the perovskites $SrTiO_3$ and $BaTiO_3$. We have performed density functional calculations within the local-orbital scheme FPLO using a recently implemented EFG module. The calculated values agree well with the experiment. We show that the electronic charge density around the oxygen ion is almost spherical for $SrTiO_3$ at the experimental volume, but surprisingly becomes more and more oblate with increasing lattice expansion. The same tendency in the density redistribution, that can be quantified as the increase of the difference in population of σ- and π- orbitals in the p shell, is found for $BaTiO_3$. Using a p-d like model Hamiltonian, we show that this counter-intuitive behavior can be explained by the contribution of oxygen $2s$ states to the crystal field on the Ti site. We argue that the surprisingly large difference between the observed electric field gradients of the two compounds in the cubic phase is mainly due to the difference in the on-site electronic density distribution. The proposed model description is of general relevance for all related transition metal oxides with similar crystal structure.

[1] R. Blinc et al. Condens. Matter **20**, 085204 (2008)

TT 31.3 Wed 16:15 HSZ 304

Experimental setup for investigation of mechanical losses of thin dielectric films at low temperatures — •Christian Schwarz[1], Stefanie Kroker[1], Ronny Nawrodt[2], Daniel Heinert[1], Stuart Reid[2], Iain Martin[2], Eleanor Chalkley[2], Ralf Neubert[1], Wolfgang Vodel[1], Andreas Tünnermann[3], Sheila Rowan[2], Jim Hough[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]University of Glasgow, Institute for Gravitational Research, Kelvinbuilding, University Avenue, G12 8QQ Glasgow, Scotland — [3]Friedrich-Schiller-Universität Jena, Institut für Angewandte Physik, Albert-Einstein-Straße 15, D-07745 Jena, Germany

Low mechanical loss materials are needed for enhanced future gravitational wave detectors in order to reduce thermal noise. The dielectric layers needed to form optical components play a crucial role. We present an experimental setup for the investigation of the mechanical losses of thin ($<1\,\mu$m) dielectric films on silicon cantilevers over a temperature range from 5 to 300 K. The experimental limits of the setup are investigated and discussed. First results on uncoated and coated cantilevers are presented. The cantilevers are coated with tantala (Ta_2O_5) by means of electron beam evaporation.

This work is in part supported by the German science foundation DFG under contract SFB TR7.

TT 31.4 Wed 16:30 HSZ 304

Effect of the spin-orbit interaction on the thermodynamic properties of Bi and Sb — •Reinhard K. Kremer[1], Manuel Cardona[1], Luis E. Díaz-Sánchez[2], Aldo H. Romero[2], Xavier Gonze[3], and Jorge Serrrano[4] — [1]Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]CINVESTAV, Departamento de Materiales, Unidad Querétaro, Querétaro, 76230, Mexico — [3]Unité de Physico-Chimie et de Physique des Matériaux Université Catholique de Louvain B-1348 Louvain-la-Neuve, Belgium — [4]ICREA-Dept. Física Aplicada, EPSC, Universitat Politécnica de Catalunya, Av. Canal Olímpic 15, 08860 Castelldefels, Spain

In the past years we have carried out a series of experiments as well as *ab initio* calculations of the dependence of the specific heat of semiconductors and insulators on T and isotopic masses. First results on the binary lead chalcogenides revealed marked differences between the calculated and the experimental heat capacities and the phonon dispersion relations. This finding raised the question of whether these discrepancies were due to the lack of spin-orbit (s-o) coupling in the *ab initio* electronic structure calculations. Using the ABINIT code which was recently extended to include s-o interaction we calculated the dispersion relations and the specific heat and compare it with our new low-temperature heat capacity measurements on Bi, Sb and PbX (X=S, Se, Te) and existing experimentally determined phonon dispersion relations. We find that agreement between measurements and calculations significantly improves when s-o interaction is included. Differences for the various investigated elements and binary systems are discussed.

TT 31.5 Wed 16:45 HSZ 304

Far-infrared measurements on multiferroic $TbMnO_3$ — •Michael Schmidt, Christian Kant, Torsten Rudolf, Franz Mayr, Joachim Deisenhofer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany

Recently multiferroics with strongly enhanced magnetoelectric effects attracted considerable attention. Especially $TbMnO_3$ gained a lot of interest, as in this compound it has been documented that spin waves can be excited by ac electric fields. This novel excitations of multiferroics have been termed electromagnons [1].

Despite extensive experimental and theoretical efforts, the microscopic origin of these excitations is strongly debated and their coupling to phonons is not fully understood. New models aiming to explain the origin of these excitations have been developed [2,3].

We performed polarization dependent far-infrared spectroscopy on $TbMnO_3$ for wavenumbers ranging from 40 cm^{-1} to 8000 cm^{-1} and temperatures from 5 K to 300 K. We followed in detail the temperature dependencies of eigenfrequencies, strengths and damping constants of all IR-active phonon modes, with the main emphasis to study the coupling of phonons to spin excitations. We provide experimental evidence that the low energy phonon modes are strongly coupled to spin excitations, a characteristic feature of spin driven ferroelectricity.

[1] A. Pimenov et al., Nature Phys. **2**, 97 (2006)
[2] Y. Takahashi et al., Phys. Rev. Lett. **101**, 187201 (2008)
[3] R. Valdés Aguilar et al., arXiv:0811.2966v1 (unpublished)