KFM 11: Dielectric, Elastic and Electromechanical Properties

Time: Tuesday 10:00–11:40 Location: EMH 025

KFM 11.1 Tue 10:00 EMH 025

Optical properties of titanium-doped lithium niobate from time-dependent density-functional theory — •Michael Friedrich[1], W. G. Schmidt[1], Arno Schindlmayr[1], and Simone Sanna[2] — [1]Department Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Lithium niobate ($LiNbO_3$) is a dielectric crystal with outstanding electro-optical properties that is widely used for optical waveguides and other commercial applications. The usage in waveguides is made possible by titanium indiffusion. Although this technique has been used for decades, the underlying microscopic processes during indiffusion and the definite lattice sites that are occupied by titanium are insufficiently known to this day.

We model the properties of pristine and titanium-doped $LiNbO_3$ from first principles. The dielectric functions are calculated within time-dependent density-functional theory, and a model long-range contribution is employed for the exchange-correlation kernel in order to account for the electron-hole binding. Our study focuses mainly on the influence of substitutional titanium atoms on lithium sites. We show that an increasing titanium concentration enhances the values of the refractive indices and the reflectivity [1]. This effect cannot be observed by titanium atoms occupying niobium sites.

[1] M. Friedrich *et al.*, Phys. Rev. Materials **1**, 034401 (2017).

KFM 11.2 Tue 10:20 EMH 025

Characterization of extremely small nonlinearities of dielectric response in glasses and glass ceramics — •Florian Bergmann[1,2], Martin Letz[1,2], Gerhard Jakob[2], and Holger Maune[3] — [1]Schott AG, Mainz, Germany — [2]Johannes Gutenberg Universität, Mainz, Germany — [3]Technische Universität, Darmstadt, Germany

Recent mobile network solutions require better microwave circuit performances than ever before. Material solutions need to tackle the challenge of intermodulation between high power signals, e.g. the sending channels of a microwave base station. Intermodulated signals can interfere with the receiving channel with orders of magnitude lower intensity. Therefore, also these very weak passive intermodulation (PIM) levels need to be controlled. One source of intermodulation is the nonlinear response of dielectrics to the electric field. However, there exists only few experimental data on the characterization of nonlinear dielectrics in the GHz frequency range with a sensitivity necessary for mobile communication solutions. Following a resonator method (1) exciting eigenresonances of three coupled cylindrical dielectric resonators enables to measure nonlinear behavior at high field strengths and allow isolating the resonators' material nonlinearities from other intermodulation sources. We report on the latest progress on determining the nonlinear response of glass and glass-ceramics.

(1) T. Nishikawa et al. 'Third harmonic distortion of dielectric resonator material' Jpn. J. Appl. Phys. 28, 2528-31, (1989).

KFM 11.3 Tue 10:40 EMH 025

Sequential polarization switching in ferroelectrics* — •Ruben Khachaturyan — Technische Universität Darmstadt, Darmstadt, Germany

The classical Kolmogorov-Avrami-Ishibashi (KAI) statistical theory of polarization reversal in a uniform ferroelectric medium proved to be a widely used tool in polarization kinetics description. However, based on independent nucleation mechanism the model is not able to describe subsequent events such as 90°-switchings which follow each other. Such 90°-switchings were established experimentally by in situ x-ray diffraction measurements and ultrasonic investigations.

In this work, we expand the KAI model to describe also sequential 90°-switchings. The model explains well recent experimental results of simultaneous time-resolved macroscopic measurements of polarization and strain, performed on a tetragonal Pb(Zr,Ti)O3 ceramic.

Results of simulation allow us to distinguish between 90°- and 180° switchings, estimate their shares as well as to determine characteristic switching times of these processes, and their activation fields.

KFM 11.4 Tue 11:00 EMH 025

Dielectric Response - Answer to Many Questions in the Methylammonium Lead Halide Solar Cell Absorbers — •Doru C. Lupascu[1], Irina Anusca[1], Šarunas Svirskas[2], Pascale Gemeiner[3], Mehmet Sanlialp[1], Gerhard Lackner[1], Christian Fettkenhauer[1], Jaroslavas Belovickis[2], Vytautas Samulionis[2], Maksim Ivanov[2], Brahim Dkhil[3], Juras Banys[2], and Vladimir V. Shvartsman[1] — [1]Universität Duisburg-Essen, Essen, Deutschland — [2]Vilnius University, Vilnius, Lithuania — [3]Centralesupelec, Gif-sur-Yvette, France

Hybrid organic-inorganic perovskites CH3NH3PbX3 (X = I, Br, Cl) can potentially revolutionize the world of solar cells. The origin of the exceptionally large diffusion length of their photogenerated charge carriers, that is, their low recombination rate, remains elusive. We show that the dielectric constant conserves very high values (>27) for frequencies below 1 THz in all three halides. This efficiently prevents photocarrier trapping and their recombination owing to the strong screening. Similarly large contributions to the dielectric constant are attributed to the dipolar disorder of the CH3NH3+ cations as well as lattice dynamics in the Gigahertz range yielding dielectric constants of $\epsilon = 62$ for the iodide, 58 for the bromide, and about 45 for the chloride below 1 GHz at room temperature. Disorder continuously reduces for decreasing temperature. Dipole dynamics prevail in the intermediate tetragonal phase. The low-temperature orthorhombic state is antipolar. No indications of ferroelectricity are found.

KFM 11.5 Tue 11:20 EMH 025

On the Theory of Magneto-Optical Effects in Crystalline Dielectrics — •Nadine Suzan Cetin, Marius Dommermuth, and Nils Schopohl — Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena and their Applications in LISA$^+$, Eberhard-Karls-Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

A recent theory of the propagation of light in crystalline dielectrics, based on an exact solution of the fundamental field integral equations determining the microscopic local electric field, solely with the individual microscopic polarizabilities $\alpha(\mathbf{R},\omega)$ of atoms (molecules, ions) at a site $\mathbf{R}$ and the crystalline symmetry as input into the theory[1], is extended to take into account the effects of a static external magnetic induction field $\mathbf{B}^{(0)}$ within a Lorentz oscillator model. Decomposing the microscopic local electric field into longitudinal and transversal parts, an effective wave equation determining the radiative part of the macroscopic field in terms of the transverse dielectric tensor $\varepsilon_{ab}^{(T)}\left(\mathbf{q},\omega;\mathbf{B}^{(0)}\right)$ is deduced from the exact solution to the field-integral equations. The Taylor expansion $\varepsilon_{ab}^{(T)}\left(\mathbf{q},\omega;\mathbf{B}^{(0)}\right) = \varepsilon_{ab}^{(T)}(\omega) + i\gamma_{abc}(\omega)\, q_c + \alpha_{abcd}(\omega)\, q_c q_d + A_{abc}^{(1)}(\omega)\, B_c^{()} + A_{abcd}^{(1)}(\omega)\, B_c^{(0)} q_d + \ldots$ around $\mathbf{q} = \mathbf{0}$ and around $\mathbf{B}^{(0)} = \mathbf{0}$ provides then insight into various optical and magneto-optical phenomena, in full agreement with the phenomenological reasoning of Agranovich and Ginzburg. We present calculations of the Faraday effect for quartz, CaF_2 and BaF_2 and compare with experimental data.

[1] Marius Dommermuth and Nils Schopohl, arXiv:1709.07277