

DF 11: Optical and nonlinear optical properties, photonic

Time: Wednesday 9:30–12:20

Location: EB 107

DF 11.1 Wed 9:30 EB 107

Dispersive properties of small polaron-based hologram recording in nominally undoped, thermally reduced LiNbO₃ — •HAUKE BRUENING and MIRCO IMLAU — Department of Physics, University of Osnabrück, Germany

We recently discovered a new type of hologram recording in nominally undoped, thermally reduced LiNbO₃ by means of a single intense ns-laser pulse ($\lambda = 532$ nm) yielding short-lived volume phase-gratings with unique features [1]: a diffraction efficiency η of more than 20% in the NIR spectral range ($\lambda = 785$ nm), a stretched-exponential relaxation behavior of the grating efficiency with a lifetime in the ms-range at room temperature, an acceleration of the decay with increasing temperature and a pronounced dependence of η on the orientation of the grating vector with respect to the polar c-axis. This type of hologram recording could be successfully modeled by taking into account an optically generated spatial modulation of small bipolarons, bound and free polarons. In this contribution, we face the unique dispersive properties of this type of hologram recording and particularly present our results for probing the gratings in the blue-green spectral range ($\lambda = 488$ nm). We show that the contribution of small bound hole polarons has to be considered as well. It can be concluded that a diffraction efficiency of about $\eta \approx 0.5 \cdot 10^{-4}$ at the telecommunication wavelength ($\lambda = 1550$ nm) can be expected.

*Financial support by the DFG (IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.

[1] M. Imlau et al., Optics Express 19, 15322 (2011)

DF 11.2 Wed 9:50 EB 107

Quantitative examination of out-of-phase mixed holographic gratings — •KAY-MICHAEL VOIT, HAUKE BRUENING, and MIRCO IMLAU — Department of Physics, University of Osnabrück, Germany

Modern holographic applications require advanced photosensitive materials that particularly obey alterations of the complex permittivity with pronounced amplitudes of both real and imaginary parts on the sub-ps-time scale. Promising candidates such as amorphous and crystalline materials remarkably show a mutual phase-shift between phase and absorption gratings that complicates the analysis of the underlying wave-coupling mechanisms. Hence, theoretical descriptions that are simply based on Kogelnik's coupled-wave theory can not be applied, i.e., a formal approach to systematically derive the full parameter space of the gratings from diffraction efficiency measurements is missing in literature. We revised the analysis of the wave-coupling theory omitting former approximations or applying them later. As a result we derived a formal description for mixed gratings allowing for a full description of beam-coupling experiments. Both the modulations of the refractive index and the absorption coefficient as well as the phase shift between these gratings can be determined through measurements of the angular dependent diffraction efficiency around the positive and the negative Bragg angle. Our approach and results are demonstrated along a mixed grating with a most common parameter set.

*Financial support by the DFG (projects IM 37/5, INST 109/137) is gratefully acknowledged.

DF 11.3 Wed 10:10 EB 107

Surface plasmon resonance of Ag nanoclusters and refractive index changes in ion irradiated lithium niobate — •JURA RENSBERG, STEFFEN MILZ, CARSTEN RONNING, and WERNER WESCH — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Lithium niobate (LiNbO₃) is one of the most important materials for integrated optics, because of its unique electro-optical and nonlinear optical properties. Ion beam synthesis plays a key role in fabricating arrays of metal nanoclusters embedded in LiNbO₃ particularly with regard to plasmonic applications. Major challenges of this technique are on the one hand to control the cluster size distribution and on the other hand to avoid irradiation damage of the LiNbO₃. Therefore we have implanted 380 keV Ag⁺ ions up to an ion fluence of $1 \times 10^{17} \text{ cm}^{-2}$ into LiNbO₃ at room temperature. As a consequence Ag clusters nucleated and a broad amorphous layer was produced. Isochronal rapid thermal annealing as well as isothermal annealing were performed in the temperature range of 573 K to 1173 K, which leads to refractive

index changes associated with lattice structure recovery.

In this contribution we shall report on polarization dependent optical spectroscopy of the surface plasmon resonance of silver nanoclusters embedded in LiNbO₃ combined with Mie theory simulations to investigate the refractive index changes upon ion irradiation and annealing.

DF 11.4 Wed 10:30 EB 107

Vergleich der optischen Materialmodifikationen von Lithiumniobat-Kristallen durch den Beschuss verschiedener schneller leichter Ionen — •JOHANNES GOETZE, NIELS L. RÄTH, KONRAD PEITHMANN und KARL MAIER — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn

Lithiumniobat-Kristalle finden vielfach Anwendung in Wissenschaft und Technik, insbesondere in optischen Technologien. Methoden zur gezielten Strukturierung wichtiger Materialparameter, wie des Brechungsindex, der elektrischen Leitfähigkeit oder der ferroelektrischen Polungseigenschaften, sind daher gefragt.

Durchstrahlung der Kristalle mit hochenergetischen leichten Ionen, wie beispielsweise ³He, ist eine leistungsfähige Methode zur Beeinflussung der Materialparameter. Da sie als Nebenwirkung eine parasitäre Aktivierung der Kristalle mit sich bringt, wird durch den Einsatz verschiedener Projektile (³He, ⁴He, ¹H, ²D) untersucht, ob eine Optimierung des Prozesses möglich ist.

Der Einfluss der Projektilwahl hinsichtlich der oben genannten Bereiche soll vorgestellt werden.

10 min. break

DF 11.5 Wed 11:00 EB 107

Finding optimal starting points for quasi-particle band structures and optical properties of transparent conducting oxides.

— •MARTIN STANKOVSKI¹, ANNA MIGLIO¹, DAVID WAROQUIERS¹, GABRIEL ANTONIUS², MATTEO GIANTOMASSI¹, MICHEL CÔTÉ², XAVIER GONZE¹, and GIAN-MARCO RIGNANESI¹ — ¹IMCN-NAPS, Université catholique de Louvain, Place Croix du Sud 1, B-1348 Louvain-la-Neuve, Belgium — ²Département de physique, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Canada H3C 3J7

We use analytic multi-pole models in lieu of standard plasmon-pole models [PRB(RC), accepted (2011)] in order to capture the detailed frequency dependence of the screened Coulomb interaction in crystalline systems [pssb 248, 275 (2011)]. These are applied in a quasi-particle self-consistent GW scheme for the evaluation of the many-body quasi-particle bulk band structure of the transparent conducting oxide hosts ZnO, MgO, SnO and SnO₂. Optical spectra obtained using the Bethe-Salpeter equation are compared with experiment and with methods utilising the orbitals and eigenenergies from computationally less demanding ground-state methods. Several current popular local and non-local ground-state DFT and generalised Kohn-Sham approaches like the LDA, GGA, meta-GGA, and COHSEX are tested in this way. These studies show that it is possible to obtain a good description of optical spectra with a reasonable computational effort.

DF 11.6 Wed 11:20 EB 107

Electronic structure of lanthanum bromide and strontium iodide from many-body perturbation theory calculations — •PAUL ERHART^{1,2}, DANIEL ÅBERG², and BABAK SADIGH² — ¹Applied Physics, Chalmers University of Technology, Gothenburg, Sweden — ²Lawrence Livermore National Laboratory, Livermore, California, USA

Rare-earth based scintillators represent a challenging class of scintillator materials due to pronounced spin-orbit coupling and subtle interactions between d and f states that cannot be reproduced by standard electronic structure methods such as density functional theory. In this contribution we present a detailed investigation of the electronic band structure of LaBr₃ using the quasi-particle self-consistent GW (scGW) method. This parameter-free approach is shown to yield an excellent description of the electronic structure of LaBr₃. Specifically we reproduce the correct level ordering and spacing of the 4f and 5d states, which are inverted with respect to the free La atom, the band gap as well as the spin-orbit splitting of La-derived states. We furthermore present electronic structure calculations using G₀W₀ for the

important scintillator material SrI_2 . We explicitly take into account spin-orbit coupling at all levels of the theory. Our results demonstrate the applicability and reliability of the scGW approach for rare-earth halides. They furthermore provide an excellent starting point for investigating the electronic structure of rare-earth dopants such as Ce and Er.

DF 11.7 Wed 11:40 EB 107

Circular Dichroism in Biological Photonic Crystals —

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We introduce a chirality index that measures the circular dichroism of chiral photonic crystals by quantifying the degree of circular polarisation of the photonic band structure eigenmodes [1]. Nature provides a variety of examples for structural color in bird feathers, beetle shells and butterfly wings. It is widely accepted that the green color of the butterfly callophrys Rubi is caused by the nanostructure of its chitin wing-scales. This structure is modelled by a Gyroid constant mean curvature body and acts as a photonic crystal [2]. Our method, backed up by an alternative numerical transmission calculation based on a scattering matrix approach, reveals strong circular dichroism of the chiral Gyroid photonic crystal in the near UV. This response is a remarkable finding for a photonic crystal made of air and chitin with a low dielectric contrast and suggests technological designs [3] as well as possible relevance for butterfly communication.

- [1] M. Saba et al., Phys. Rev. Lett. 106, 103902 (2011)
- [2] G.E. Schröder-Turk et al., J. Struct. Biol. 174(2), 290 (2011)
- [3] M. D. Turner et al., Opt. Express 19, 10001 (2011).

DF 11.8 Wed 12:00 EB 107

Aufbau eines NOPA bei 208 kHz Wiederholrate für Röntgen-Pump-Probe Experimente am Synchrotron — •MATHIAS SANDER, HENGAMEH NAVIRIAN, PETER GAAL und MATIAS BARGHEER —

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Wir verwenden einen nicht-kollinearen phasenangepassten optisch parametrischen Verstärker (NOPA) [1], der von einem faserbasierten Lasersystem mit einer einstellbaren Repitionsrate zwischen 200 kHz bis 25 MHz gepumpt wird, für hochsensitive Anrege-Abtast-Experimente. Das Lasersystem ist als Anregequelle für zeitaufgelöste Röntgendiffraktionsexperimente am Synchrotron BESSY II konzipiert. Die Emissionswellenlänge des Lasers von 1035 nm wird direkt zur Erzeugung eines Weißlicht-Kontinuums in einem Saphir-Kristall verwendet. Im weiteren mehrstufigen Aufbau können so durchstimmbare Laserpulse im Bereich von 620 nm bis 970 nm erzeugt werden. Durch anschließende Wellenlängenkonversion dieser Pulse mittels zweiter und dritter Harmonischen sowie Summenfrequenzmischung lassen sich sogar Wellenlängen deutlich unter 300 nm erreichen. In diesem NOPA-Aufbau lassen sich Pulsdauern unter 20 fs bei Pulsenergien von ca. 850 nJ erreichen. Die Sensitivität des Aufbaus soll durch hochrepetitives scannen gesteigert werden. Zukünftig soll der Aufbau in Verbindung mit der Synchrotronquelle zur Untersuchung von nanostrukturierten Schichtsystemen und komplexen Materialien, z.B. Perovskit-Oxiden, verwendet werden.

- [1] E. Riedle et al., Optics Letters Vol. 33, No.2 (2008)