

## KFM 16: Crystal Structure Defects / Real Structure / Microstructure I

Chair: Theo Scherer (KIT Karlsruhe)

Time: Wednesday 15:00–17:10

Location: E 124

KFM 16.1 Wed 15:00 E 124

**Ultrafast laser induced structural motion in crystalline and amorphous gold** — ●OTHMANE BENHAYOUN<sup>1</sup>, EMILIANO PRINCIPPI<sup>2</sup>, BERND BAUERHENNE<sup>3</sup>, DMITRY IVANOV<sup>4</sup>, and MARTIN GARCIA<sup>1</sup> — <sup>1</sup>University of Kassel, Theoretical physics II, Kassel, Germany — <sup>2</sup>Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy — <sup>3</sup>University of Kassel, Theoretical physics I, Kassel, Germany — <sup>4</sup>Moscow, Russia

An Ultrafast Electron Diffraction (UED) experiment showed a time-dependent nonuniform compression and expansion of a monocrystalline gold foil. This led to the time modulation of the Au Bragg peaks in both height and width that was measured by the experiment. The same effect is however not observed in polycrystalline gold. We thus perform Molecular Dynamics - Two Temperature Model (MD-TTM) simulations aiming to understand the results of the experiment. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics in the monocrystalline case and compare them with the polycrystalline case.

KFM 16.2 Wed 15:20 E 124

**Laser-assisted formation of local defined absorbers for Cu(In,Ga)Se<sub>2</sub>-micro-concentrator solar cells** — ●SETAREH ZAHEDI AZAD<sup>1</sup>, OWEN.C. ERNST<sup>1</sup>, TORSTEN BOECK<sup>1</sup>, HEIKE VOSS<sup>2</sup>, SONJA CINQUE<sup>2</sup>, JÖRN BONSE<sup>2</sup>, JÖRG KRÜGER<sup>2</sup>, JAN LUCASSEN<sup>3</sup>, MARTINA SCHMID<sup>3</sup>, and JENS MARTIN<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, 12489, Germany — <sup>2</sup>Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany — <sup>3</sup>Universität Duisburg-Essen, Forsthausweg 2, 47057 Duisburg, Germany

The micro-concentrator design for high-performance Cu(In,Ga)Se<sub>2</sub> (CIGSe) solar cells is a promising approach to reduce the consumption of Indium and Gallium [1]. To save these rare materials, the local nucleation of (In,Ga)-islands at a micrometre scale is investigated. Our results show that the selective formation of an array of indium and gallium islands on Mo-coated soda-lime glass substrates is possible using localized laser-heating by a cw-laser, a diffractive optical element (DOE), and the use of trimethylindium and triethylgallium as precursors. The results indicate that nucleation is dependent on the laser power and the roughness of Molybdenum. By evaporation of Copper in a PVD chamber followed by selenization, the (In,Ga)-islands turn to CIGSe-islands serving as absorbers for micro-concentrator solar cells. Since the size and pattern of the CIGSe-islands can be easily controlled using the laser-heating/DOE-setup, this novel method can also be applied to large-scale production. [1] Sadewasser, S., Solar Energy 158 (2017): 186-191.

KFM 16.3 Wed 15:40 E 124

**Influence of Ga concentration on crystal structure of CoCrFeNiGa<sub>x</sub> (x = 0.5, 1) high-entropy alloys** — ●TATIANA SMOLJAROVA<sup>1</sup>, IVAN TARASOV<sup>1</sup>, MARINA SPASOVA<sup>1</sup>, ANDRÁS KOVÁCS<sup>2</sup>, RAFAL E. DUNIN-BORKOWSKI<sup>2</sup>, MICHAEL FARLE<sup>1</sup>, and NATALIA SHKODICH<sup>1</sup> — <sup>1</sup>Faculty of Physics and Center for Nanointegration, Universität Duisburg-Essen, Duisburg, Germany — <sup>2</sup>Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany

High-entropy alloys (HEAs) offer a novel approach to explore multi-component phase diagrams, leading to the discovery of new materials. Here, we report a transmission electron microscopy (TEM) study of the structural changes observed in micro-sized CoCrFeNiGa<sub>x</sub> (x = 0.5, 1.0) powders, prepared by high-energy ball milling (HEBM) in planetary ball mills at room temperature. The process results in the formation of an FCC crystal structure and compositional homogeneity. Additionally, we find in bulk samples obtained by consolidating the prepared micropowder using the spark plasma sintering (SPS) process (1073 K) preferential fcc structure for the CoCrFeNiGa<sub>0.5</sub> powder, and a partial transformation of the FCC into a BCC structure for the equiatomic CoCrFeNiGa powder. Financial support by DFG, CRC/TRR 270 (project ID 405553726) is acknowledged.

10 min. break

KFM 16.4 Wed 16:10 E 124

**Temperature-dependent Peierls Distortion in the Phase Change Material In<sub>3</sub>SbTe<sub>2</sub>** — ●MARIA HÄSER<sup>1</sup>, MARTIN ETTER<sup>2</sup>, HENRIK JEPPESEN<sup>2</sup>, SEBASTIAN GEISLER<sup>3</sup>, OLIVER OECKLER<sup>3</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>I. Institute of Physics (IA), RWTH Aachen University, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — <sup>3</sup>Faculty of Chemistry and Mineralogy, Institute of Mineralogy, Crystallography and Materials Science, Leipzig University, Germany

In recent years, interest in chalcogenide-based phase change materials (PCMs) has increased in photonic applications due to their significant difference in optical properties between the amorphous and crystalline phases. A promising candidate for photonic devices is In<sub>3</sub>SbTe<sub>2</sub> (IST), which is a plasmonic PCM with metallic properties in the crystalline phase and semiconducting properties in the amorphous state. Using synchrotron radiation, the temperature-dependent atomic arrangement of crystalline IST has been investigated. The simulation of measured Powder X-Ray Diffraction (P-XRD) and Pair Distribution Function (PDF) data allows a direct comparison of the average and the local atomic arrangement: Although IST crystallizes in NaCl structure type (space group Fm-3m (225)) on average, we report local deviations from this structure. These Peierls-like deviations increase with increasing temperature. This finding can explain the temperature dependent behavior of IST and similar materials.

KFM 16.5 Wed 16:30 E 124

**Where is the hydrogen going? – An investigation of lithium metal oxides** — ●THOMAS KÖHLER<sup>1</sup>, MATTHIAS ZSCHORNAK<sup>1</sup>, PATRICK REICHART<sup>2</sup>, ERICA BRENDLER<sup>1</sup>, CHRISTIAN RÖDER<sup>1</sup>, GÜNTHER DOLLINGER<sup>2</sup>, HARTMUT STÖCKER<sup>1</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>TU Bergakademie Freiberg, 09599 Freiberg, Germany — <sup>2</sup>Universität der Bundeswehr München, 85579 Neubiberg, Germany

The incorporation of hydrogen into LiNbO<sub>3</sub> and LiTaO<sub>3</sub> during crystal growth has attracted the interest of researchers for more than 50 years. Our studies address the following open points: (i) the model description of the occupation sites, (ii) the diffusion kinetics, and (iii) the hydrogen concentration determination. Hydrogen bonds to oxygen and forms hydroxyl (OH<sup>-</sup>) defects. Since the shape of the vibrational modes strongly depends on the crystal stoichiometry, we can use them to elucidate the presence of different hydrogen occupation sites and the associated chemical environment.

Experimental and theoretical studies indicate that the intrinsic and extrinsic defects of the crystals are crucial, as hydrogen only decorates these defects. The diffusion of hydrogen was studied using elevated temperatures and different atmospheric conditions. Differences in diffusion rate and activation energy are dependent on the dominating defect type. Finally, the question arises: What is the natural hydrogen concentration in these materials? Hydrogen microscopy using proton-proton scattering is found to be the only reliable tool for absolute quantification and can be applied to obtain a calibration factor for infrared spectroscopy.

KFM 16.6 Wed 16:50 E 124

**Evaluation of structural phase transition in spin-1/2 frustrated Dirac-magnon antiferromagnet: Cu<sub>3</sub>TeO<sub>6</sub>** — ●ISHA ISHA<sup>1</sup>, M. ISOBE<sup>2</sup>, N. P. LALLA<sup>1</sup>, and ARVIND KUMAR YOGI<sup>1</sup> — <sup>1</sup>UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — <sup>2</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We report the structural and physical properties of spin-1/2 ( $3d^9$  as  $Cu^{2+}$ ) ultra-high quality single-crystals of Cu<sub>3</sub>TeO<sub>6</sub>. The susceptibility measured over single-crystal is showing quasi-1D behavior as confirmed by using Bonner-Fisher spin-1/2 1D chain model in the temperature range from 20 K to 200 K. From magnetic susceptibility we deduce the nearest neighbor (NN) antiferromagnetic coupling constant  $J \sim 113.2$  K. We show that this compound made of weakly coupled infinite chains of CuO<sub>6</sub> octahedral. Moreover, we have performed detailed x-ray diffraction technique to elucidate a structural-phase transition and our detailed analysis suggests an isostructural transition, resulting in an unusually temperature dependence of cubic cell parameter and

atomic displacement below the second-order phase transition ( $T_N \sim 61$  K) which indicates strong magneto-elastic coupling. Our results re-

veal yet another interesting facet of the magneto-elastic coupling in the  $\text{Cu}_3\text{TeO}_6$  spin-web lattice.