KFM 8: Crystallography in Materials Science, Microstructure and Dielectric Properties

Time: Monday 15:00–17:15 Location: H7

KFM 8.1 Mon 15:00 H7

In Situ Structural and Optical Characterization of Laser Recrystallization in an Ultrafast TEM — •Jakob Hagen, Murat Sivis, and Claus Ropers — Max-Planck-Institute for Multidisciplinary Sciences, Göttingen, Germany

Surface-plasmon resonances (SPR) have gained increasing attention due to their widespread use in various scientific fields [1]. These resonantly excited collective free-electron oscillations are able to localize and enhance electromagnetic fields beyond the diffraction limit [2]. To this date, the fabrication of such structures with high optical quality remains challenging, since in general, bottom-up-approaches suffer from the poly-crystallinity of the metal which counteracts the plasmon propagation by damping at grain boundaries [3]. In this study, we created plasmonic nanodiscs by electron beam lithography (EBL) and subsequently performed in situ annealing with a pulsed laser source in an ultrafast transmission electron microscope (TEM). This method allows for live-tracking of the boundary migration and also for characterization of SPRs by photon-induced near-field electron microscopy (PINEM) [4]. Upon illumination, the number of grains reduces drastically leading to almost perfect mono-crystals while preserving the shape. Our approach combines the benefits of mono-crystalline plasmonics [5] with nanometrically precise positioning from EBL.

[1] S. Lal et al., Nat. Photonics 1, 641-648 (2007), [2] K. B. Crozier et al., J. Appl. Phys., 94, 4632 (2003), [3] M. Bosman et al., Sci. Rep. 4, 5537 (2014), [4] L. Piazza et al., Nat. Commun. 6, 6407 (2015), [5] J.-S. Huang, Nat. Commun., 1:150 (2010)

KFM 8.2 Mon 15:20 H7

Impact of the stacking sequence on the stability of transition-metal diborides — •Thomas Leiner[1], Nikola Koutná[2], Paul H. Mayrhofer[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Austria — [2]Institute of Materials Science and Technology, TU Wien, Austria

Transition-metal diborides are a very hard and brittle type of materials, which, among others, find their use as protective coatings, because of their excellent heat conductivity, oxidation stability and wear resistance.

The investigated diborides XB_2 X=(Cr, Hf, Mn, Mo, Nb, Re, Ta, Ti, V, Zr) occur in three different known stackings, the A-A-A-A stacking of e.g. TiB_2, the A-B-A-B stacking of ReB_2 and the A-B-B-A stacking of WB_2.

In this work, the impact of the stacking sequence on the stability of diborides is investigated via *ab initio* methods (VASP) and phonon analysis. The energy levels and the energy barriers for the different structures of the transition-metal diborides is calculated and evaluated. The stability of observed local and global energy minima are further investigated by assessing their phonon density of states and their phonon frequencies.

Predictions about a possible stability of certain stackings are made and the behaviour of different diborides was compared to each other.

KFM 8.3 Mon 15:40 H7

Pressure-driven insulator-to-metal transition and superconductivity in one-dimensional transition-metal-trichalcogenide microstructures — •Chin Shen Ong[1], L. F. Shi[2,3], Jin-Guang Cheng[2,3], Irina Gorlova[4], Sergey Zybtsev[4], Lingyi Ao[5], Junwei Huang[5], Hongtao Yuan[5], Raman Thiyagarajan[6], Vadim Pokrovskii[4], Olle Eriksson[1,7], and Mahmoud Abdel-Hafiez[1] — [1]Uppsala University, Uppsala, Sweden — [2]Chinese Academy of Sciences, Beijing, China — [3]University of Chinese Academy of Sciences, Beijing, China — [4]Moscow — [5]Nanjing University, Nanjing, China. — [6]Indian Institute of Technology Madras, Chennai, India — [7]Örebro University, Örebro, Sweden

Transition metal trichalcogenides exhibit large tunability of nontrivial electronic states by modifying chemical composition, temperature, and pressure. Despite great interest in TMTCs, very little information exists on how their electronic properties change with compression. Here, we systematically investigate the high-pressure behavior of n-type semiconducting TiS3 of one-dimensional microstructural form. High-pressure electrical resistance measurements up to 98 GPa identify an exotic sequence of transitions from being a semiconductor to insulator, then metal and finally, a hitherto undiscovered superconducting phase at pressures above 70 GPa. The experimental results are supported by first-principles theoretical calculations.

KFM 8.4 Mon 16:00 H7

Impact of point defects on the ferroelectric phase diagram: a molecular dynamics study on the defect arrangements — •Sheng-Han Teng and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Ferroelectric perovskites usually host imperfections and defects that affect their functional properties. Aging and fatigue are often related to the redistribution of these defects [1-3]. Microscopic insights are therefore needed to better apply these materials to different applications. In this study, we use the first-principle based effective Hamiltonian method [4] to screen the impact of distribution and agglomeration of point defects on the phase diagrams of $BaTiO_3$-based materials. With this approach, we can simulate up to 10^6 unit cells and efficiently investigate different defect arrangements. We find that the local fields induced by the defect dipoles play a key role in ferroelectric phase stability and the optimization of functional properties.

[1] Yuri A. Genenko, Julia Glaum, Michael J. Hoffmann, and Karsten Albe. *Mater. Sci. Eng. B*, **192**, 52-82 (2015)

[2] D. Lupascu and J. Rödel. *Adv. Eng. Mater.* **7**(10), 882-898 (2005)

[3] Xiaobing Ren. *Nat. Mater.* **3**(2), 91-94 (2004)

[4] T. Nishimatsu, A. Grünebohm, U. V. Waghmare, M. Kubo, *J. Phys. Soc. Jpn.* **85**, 114714 (2016)

15 min. break

KFM 8.5 Mon 16:35 H7

Strain-Induced Collapse of Landau Levels in TaAs — •Yang-Jun Lee[1,2,3], Cheol-Hwan Park[1,2,3], and Maria A.H Vozmediano[4] — [1]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, Madrid 28049, Spain

A Weyl semimetal, which has a topologically protected conic electronic structure, hosts interesting phenomena such as Fermi arc surface states and chiral anomaly. Recently, the deformation-driven pseudo gauge fields in strained Weyl semimetals have received attention. Among such examples is the collapse of strain-induced Landau levels in Weyl semimetal. In this study, we establish the theory for the effect of strain-induced gauge fields on realistic Weyl semimetals, and based on first-principles calculations, we investigate the conditions on the external strain for the collapse of Landau levels in TaAs.

KFM 8.6 Mon 16:55 H7

Hidden order in ferroelectric oxide thin films — •Joohee Bang[1], Nives Strkalj[2], Martin Sarott[1], Morgan Trassin[1], and Thomas Weber[1] — [1]Department of Materials Science, ETH Zurich, Zurich, Switzerland — [2]Department of Materials Science and Metallurgy, Cambridge University, Cambridge, United Kingdom

Nontrivial polar topologies such as flux-closure, vortex-antivortex pair, and skyrmions in ferroelectric thin films have recently garnered much interest as they have implications for the creation of new states of matter and hold promise for alternative device configurations for microelectronics [1]. These observations called for an in-depth structural investigation of the material as the polarization states such as orientation and domain architecture define the macroscopic ferroelectric properties in ferroelectric thin films. In fact, characterization of local order in such films using noninvasive probes is important as it not only allows access to the polarization states in the bulk, but also tracks structural local order. Here, we present a newly discovered local order state on ferroelectric lead titanate and dielectric strontium titanate superlattices from a comprehensive reciprocal space investigation analyzed with three-dimensional delta pair distribution function (3D-ΔPDF) method [2]. The structural analysis was performed by collecting a complete three-dimensional diffuse X-ray scattering data, which, to the best of our knowledge, was used for the first time to study local order in single-crystalline thin films.

[1]Yadav, A., et al. 2016
[2]Weber and Simonov 2012