

KFM 11: Crystal Structure Defects / Real Structure / Microstructure

Time: Tuesday 9:30–11:10

Location: H7

KFM 11.1 Tue 9:30 H7

HRTEM study of nanoparticle precipitation in additively manufactured 1.2709 maraging steel — ●ANNA BENEDIKTOVÁ¹, DAGMAR JANDOVÁ¹, JIŘÍ BENEDIKT², ROSTISLAV MEDLÍN¹, and JÁN MINÁR¹ — ¹New Technologies - Research Center, University of West Bohemia, Pilsen, Czech Republic — ²Faculty of Applied Sciences, University of West Bohemia, Pilsen, Czech Republic

Maraging steels are known for their excellent properties, such as high strength and toughness, which are mainly due to the precipitation of intermetallic compounds during heat treatment. Up to now, mainly precipitation hardening from a temperature of about 500 °C has been studied, however, the hardening effect begins to show clearly at lower temperatures, even from 250 °C.

The HRTEM study was performed on maraging steel samples without tempering as well as after tempering at 350 °C and 490 °C, and the results were compared with simulations. Besides other relatively coarse precipitates, a high density of globular coherent nanoparticles with a superlattice was found in samples tempered at 350 °C. While the sample tempered at 490 °C contained slightly larger globular and rod-shaped Ni3Mo particles.

KFM 11.2 Tue 9:50 H7

Tuning local structure in Prussian Blue Analogues — ●YEVHENIIA KHOLINA and ARKADIY SIMONOV — ETH Zurich, Switzerland

Prussian Blue analogues, $M[M'(CN)_6]_{1-x} \cdot nH_2O$, which we abbreviate here as $M[M']$ (M and M' =transition metal ions), is a diverse family of cyanide materials, which is intensely investigated for its potential application for hydrogen storage, as catalysts and as electrode materials. Applications that require efficient mass transport utilize the ability of the structure to accommodate a large number of $M'(CN)_6$ vacancies, which create a highly connected porous network. It was theoretically shown that the connectivity and the accessible volume of such a network depend on the local structure[1]. Therefore, to optimize mass transport properties not only the number of vacancies but also their distribution must be precisely controlled. In this work we show how to tune the local structure of $Mn[Co]$ Prussian Blue analogues grown in gel by varying the crystallization parameters: the type of gel, the crystallization temperature, the concentration of reactants, and the concentration of chelating agents. We probe the defect distribution by single-crystal x-ray diffuse scattering, which allows quantitative characterization of the local structure. All of the above-mentioned parameters allow smooth continuous control of diffuse scattering and thus of the local order in $Mn[Co]$ crystals.

[1] Simonov, Arkadiy, et al. "Hidden diversity of vacancy networks in Prussian blue analogues." *Nature* 578.7794 (2020): 256-260.

KFM 11.3 Tue 10:10 H7

Electronically driven anharmonicities in low-energy lattice models: Affordable molecular dynamics of charge-density-wave systems — ARNE SCHOBERT¹, ●JAN BERGES¹, MICHAEL SENTEF², MARIANA ROSSI², ERIK VAN LOON³, SERGEY BRENER⁴, and TIM WEHLING⁴ — ¹University of Bremen, Bremen, Germany — ²Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ³Lund University, Lund, Sweden — ⁴University of Hamburg, Hamburg, Germany

Charge-density waves (CDWs) occupy an important position in the phase diagram of low-dimensional systems such as the transition metal dichalcogenide monolayers. Although a CDW can often be identified

already from the undistorted structure in linear response, anharmonic effects are eventually responsible for the stabilization of the distorted phase and its precise properties. To study the mechanisms responsible for the anharmonicity, we build an ab-initio low-energy lattice model, which reproduces Born-Oppenheimer potential surfaces from density-functional-theory (DFT). The ab-initio low-energy lattice model is used for molecular dynamics in the CDW phase of 1H-TaS2.

KFM 11.4 Tue 10:30 H7

Ab Initio Thermodynamics for Surface Motifs of the M1 Selective Oxidation Catalyst — ●K. NAM¹, Y. LEE¹, L. MASLIUK², T. LUNKENBEIN², A. TRUNSCHKE², C. SCHEURER¹, and K. REUTER¹ — ¹Theory Dept., Fritz-Haber-Institut der MPG, Berlin — ²Inorganic Chemistry Dept., Fritz-Haber-Institut der MPG, Berlin

The activity and selectivity of heterogeneous catalysts can be altered noticeably by small changes in different factors such as bulk composition, dopants, defects, reaction conditions, etc. The effects of these factors are furthermore interrelated in non-trivial ways. As an important first step to rationally disentangle them, we here aim to understand their influences on the local atomic-scale structural motifs offered by the catalyst. Specifically, we do this for the M1 structural modification of $(Mo,V)O_x$ and $(Mo,V,Te,Nb)O_x$ as an active catalyst for the oxidative dehydrogenation reaction of ethane to ethylene.

The large primitive cell of this M1 catalyst challenges a detailed study by means of predictive-quality first-principles calculations. To this end, we deconstruct the primitive cell into 'rod-like structures' of surface motifs with various oxygen content, faithfully modeling reported data from electron microscopy [1]. *Ab initio* thermodynamics then allows us to explore the effect of varying reaction conditions on the stability of these motifs and thus on M1 catalyst surfaces. Exploiting the data thus generated to train a machine-learn potential we can specifically rationalize the influence of vanadium and niobium doping on the active surface structure.

[1] L. Masliuk *et al.*, *J. Phys. Chem. C* **121**, 24093 (2017).

KFM 11.5 Tue 10:50 H7

Raman spectroscopic structure analysis of colloidal semiconductor core-shell quantum dots for the achievement of near-unity quantum efficiency — ●SANDRA HINZ^{1,2}, SONJA KROHN^{2,3}, HANNES VAN AVERMAET⁴, ZEGER HENS⁴, JAN STEFFEN NIEHAUS³, JANINA MAULTZSCH¹, and HOLGER LANGE² — ¹Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — ²Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany — ³Fraunhofer IPA - Center for Applied Nano-Technology CAN, Hamburg, Germany — ⁴Physics and Chemistry of Nanostructures, Ghent University, Ghent, Belgium

State of the art applications of quantum dots (QDs) require near-unity photoluminescence quantum yield (PLQY). This demand is rarely achieved and therefore the synthesis process is under constant optimization and nanocrystals consisting of a core with one or more shells of different materials are paving the way to achieve high PLQY. As those components have diverse lattice parameters, the induction of strain within the QDs is inevitable. Recently, we applied Raman spectroscopy for in depth structure characterization and a strain minimization approach to optimize the synthesis of $InP/ZnSe/ZnS$ QDs towards near-unity PLQY. A similar effect plays a role in $CdSe/CdS$ QDs when aiming for high PLQY. In these QDs, the formation of an alloyed interface between the $CdSe$ core and CdS shell is assumed. By Raman spectroscopy, we are able to monitor the formation of these alloyed domains for different QD parameters and correlate it with the PLQY.