MM 11: Structurally and Chemically Complex Alloys

Time: Tuesday 10:15–11:45 Location: SCH/A215

MM 11.1 Tue 10:15 SCH/A215

Quantifying chemical short-range order in Ti–Zr–Nb alloys — Yujun Zhao[1,2], Andrea Fantin[3], Yue Li[1], Tong Li[2], and •Yilun Gong[4] — [1]Max-Planck-Institut für Nachhaltige Materialien, Düsseldorf, Germany — [2]Ruhr Universität Bochum (RUB), Bochum, Germany — [3]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [4]University of Oxford, Oxford, UK

Chemical short-range order (CSRO) is expected to influence phase stability and defect interactions in Ti–Zr–Nb alloys, yet its direct quantification in equiatomic TiZrNb has remained unresolved. Here, we apply X-ray absorption spectroscopy (XAS) and X-ray pair-distribution-function (PDF) analysis to experimentally probe local chemical environments in single-phase bcc TiZrNb. Nanometre-scale compositional fluctuations and elemental pair distributions are further explored using orientation-specified atom-probe tomography (APT). XAS and PDF measurements reveal small but systematic local distortions in element-specific partial coordination shells (from XAS), consistent with emerging CSRO, and ensemble-averaged structural distortions in the atomic network (from PDF). To interpret these findings, we develop density functional theory-trained interatomic potentials and perform on-lattice Monte Carlo simulations to obtain the temperature-dependent equilibrium CSRO pair correlations. Together, these results provide the first quantitative CSRO map for TiZrNb, capturing its temperature and crystallographic dependence. This establishes TiZrNb as a reference system for understanding how CSRO influences phase stability, interstitial accommodation, and mechanical behaviour in refractory alloys.

MM 11.2 Tue 10:30 SCH/A215

Radiation Tolerance in High Entropy Alloys — •Jyoti Verma[1], Paul Chekhonin[2], Andreas Worbs[1], Cornelia Kaden[2], Maciej Oskar Liedke[3], and Gregor Hlawacek[1] — [1]Institute of Ion Beam Physics and Material Research,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [2]Institute of Resource Ecology,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [3]Institute of Radiation Physics,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400

High-entropy alloys (HEAs), or compositionally complex alloys (CCAs), are near-equiatomic multicomponent materials forming single-phase solid solutions with exceptional mechanical strength, thermal stability, and radiation resistance, making them strong candidates for structural use in advanced nuclear systems. In Generation IV fission and future fusion reactors, materials must endure 500*600 °C, high neutron fluxes, and helium and hydrogen generated by 14 MeV neutrons, which significantly influence irradiation-induced defect evolution. We are investigating the irradiation response of Co-free (CrFeMnNi) CCAs using Fe-ion irradiation at 300°C to 1, 3, and 10 dpa. Transmission electron microscopy revealed typical dislocation loops, while positron annihilation spectroscopy identified vacancy-type defects and vacancy-dislocation complexes, whose concentration decreased with dose, suggesting progressive interaction and annihilation between vacancies and dislocations at higher irradiation levels. These results demonstrate the promising irradiation tolerance of Co-free CCAs for structural use in next-generation reactors.

MM 11.3 Tue 10:45 SCH/A215

Preparation of an impurity-free quinary alloy surface without significant changes in composition — •Yong-He Pan[1], Niklas Osterloh[1], Wun-Chang Pan[1], Natalia Pukhareva[2], Alfred Ludwig[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany — [2]Centre for Interface-Dominated High-Performance Materials (ZGH), Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Compositionally Complex Solid Solutions (CCSSs) are a promising new pathway to electrochemical catalysts [1,2]. Their complex surface offers multiple adsorption sites for different reaction steps simultaneously [3]. We investigated the composition of the surface elements and impurities using X-ray photoelectron spectroscopy. The quinary alloy sample Ag-Au-Ir-Pd-Pt was prepared in ultra-high vacuum by argon sputtering and annealing. Surface impurities were removed by sputtering, and the alloy composition remained stable even during prolonged thermal treatment. Optimal sputtering and annealing parameters for achieving a clean surface were established. This study clarifies the effects of these processes on the surface composition ratio of Ag-Au-Ir-Pd-Pt alloys.

[1] H. J. Qiu et al., J. Mater. Chem. A, 2019, 7, 6499 [2] T. Löffler et al., Angew. Chem. Int. Ed. 2021, 60, 26894 [3] J. K. Pedersen et al., ACS Catal. 2020, 10, 2169

MM 11.4 Tue 11:00 SCH/A215

Effect of partial occupancy on the properties of FeCr σ-phase — •Mariano Forti[1], Guillaume Laplanche[1], Wenhao Zhang[2], Ralf Drautz[1], and Thomas Hammerschmidt[1] — [1]Ruhr Universität Bochum, Germany — [2]LINK, CNRS-Saint-Gobain- NIMS

The σ-phase forms in Fe-Cr alloys over 870K at about 50 at.% Cr, strongly affecting their performance. Atomistic studies usually assume a sublattice model, but experiments show fractional occupancy of the Whyckoff sites, creating many possible local atomic configurations. This complexity limits direct sampling with DFT and opens questions about the effect of partial occupancy on properties of the σ-phase.

We address the problem using a combination of DFT and MLIPs for a $Fe_{16}Cr_{14}$ σ-phase with experimentally observed site occupancy. We use a GRACE potential to screen all possible configurations of the intermetallic and validate the predictions with DFT calculations of a representative selection of configurations.

This approach enables a direct comparison between the traditional sublattice models and explicit disorder. Our results show that partial occupancy stabilizes the σ-phase, while mechanical properties differ roughly 10% from those predicted by sublattice models.

These findings provide a clearer picture of the local chemical disorder effects on the mechanical response of the σ-phase.

MM 11.5 Tue 11:15 SCH/A215

Accurate temperature-dependent Gibbs free energies of point defects in B2 MoTa — •Xiang Xu[1], Xi Zhang[1], Sergiy V Divinski[2], and Blazej Grabowski[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Universität Münster, Münster, Germany

Controlling order-disorder motifs is proven to be a key strategy for tuning performance in complex concentrated alloys. To this end, understanding ordered configurations is particularly important, as they represent the theoretical boundary of atomic diffusion, phase stability, and order-disorder phenomena. Since point defects like vacancies and antisites control diffusion and thereby affect ordering and phase evolution, their thermodynamic properties provide critical insight into the fundamental mechanisms behind property tuning. However, difficulties in stabilizing highly ordered refractory phases and the computational complexity of finite-temperature free energy calculations have limited quantitative understanding of their defect thermodynamics. To address this gap, we employ first-principles methods to investigate vacancy thermodynamics in the prototype B2-ordered MoTa alloy systematically. By explicitly accounting for electronic excitations and thermal vibrational contributions, particularly the explicit anharmonicity, we reveal distinct temperature-dependent Gibbs energies for vacancies and antisites in the B2-ordered MoTa. Vibrational pair distribution analysis, performed using an accurate machine-learning potential, demonstrates that the difference in thermal contributions arises from the vibrational phase spaces of the investigated point defects.

MM 11.6 Tue 11:30 SCH/A215

Modelling Bulk and Confined High-entropy Materials — •Chen-Chen Er[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden Rossendorf, Dresden

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic, mechanical, and thermal properties that are promising for applications in the energy and electronics sectors. HEMs include disordered ceramics such as carbides, nitrides, or oxides with ordered anion sublattices and disorder on the metal cation sites. Generally, five or more cation species are required to maximize configurational entropy.

In our work, efficient modelling of the disordered systems is conducted based on an ensemble of ordered structures as implemented in the partial occupation algorithm (POCC) [1] within the AFLOW framework [2,3]. Predictive descriptors including the entropy forming ability (EFA) [4] and disordered enthalpy-entropy descriptor (DEED) [5] are crucial to assess synthesizability. Here, we present new results for several bulk and confined high-entropy ceramics.

[1] K. Yang *et al.*, Chem. Mater. **28**, 6484 (2016).
[2] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[3] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[4] P. Sarker *et al.*, Nat. Commun. **9**, 4980 (2018).
[5] S. Divilov *et al.*, Nature **625**, 66 (2024).