MM 42: Topical session: Data driven materials design - high through-put

Time: Wednesday 12:00–13:15 Location: BAR 205

Topical Talk MM 42.1 Wed 12:00 BAR 205

Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials — •Alfred Ludwig — Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum

The design of new materials is a key challenge in materials science: e.g. new materials for future energy systems are urgently needed. Thin film combinatorial materials science (CMS) enables an efficient generation of consistent and large datasets on (unexplored) multinary materials systems, which promotes the discovery and optimization of new materials. CMS comprises the fabrication and processing of thin film materials libraries by combinatorial sputter deposition processes and optional post-deposition treatments, followed by extensive high-throughput characterization of the thin film samples contained in these libraries. The large datasets which are produced by the combinatorial approach need to be analyzed with new software tools, e.g. for the rapid mapping of phase diagrams. Obtained results for ternary and quaternary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of the combinatorial development of intermetallic materials for superalloys and thermoelectric applications as well as the development of metal oxide thin film materials libraries for solar water splitting.

MM 42.2 Wed 12:30 BAR 205

Towards multi-scale high-throughput calculations of thermal and mechanical properties in transition-metal alloys — •Alessandro Lunghi, Stefano Sanvito, and David D. O'Regan — School of Physics, CRANN and AMBER, Trinity College Dublin, Dublin 2, Ireland

The discovery of advanced materials with targeted properties is a long-standing challenge, where computational material science is adopting an increasingly central role in establishing stable stoichiometries and property trends. The high-throughput approach is a particularly promising strategy [1], involving the calculation of specific properties of interest over combinatorial numbers of crystallographic structures. In this work, we demonstrate the high-throughput simulation of the mechanical properties for binary alloys of the form $Au_{1-x}M_x$, where M is a generic transition metal element. We have used the AFLOW repository [2] to generate more than 5000 equilibrium structures, from which we have re-relaxed and calculated the complete elastic tensor using Quantum Espresso [3]. We also show preliminary results on the development of a new methodological framework, in which, for example, the large data corpus produced during the latter screening initiative have been used to optimize empirical force fields suited for the calculation of thermal properties. This tool opens up the new possibility of extend high-throughput methods beyond system size limits of conventional DFT. [1] S. Curtarolo, et al., Nat. Mat.,12, 191-201 (2013) [2] G. L. W. Hart, et al., Phys. Rev. X 3, 041035 (2013) [3] P. Giannozzi, et al., J.Phys.:Condens.Matter, 21, 395502 (2009)

MM 42.3 Wed 12:45 BAR 205

High throughput modelling of novel borides — •David Holec[1], Vincent Moraes[2], Mirjam Arndt[3], Peter Polcik[4], and Paul Mayrhofer[5] — [1]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [2]Christian Doppler Laboratory for Application Oriented Coating Development at the Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [3]Oerlikon Balzers, Oerlikon Surface Solutions AG, Balzers, Liechtenstein — [4]Plansee Composite Materials GmbH, Lechbruck am See, Germany — [5]Institute of Materials Science and Technology, TU Wien, Vienna, Austria

Recently, computationally-driven understanding and exploring of materials have gained a lot of attention. One very prominent example of the fruitful symbiosis between theory and experiment is protective coatings based on nitrides. There, modelling serves as a reliable trend-giver and often provides also quantitative predictions.

In the quest of exploring new hard materials, we employ high-throughput *ab initio* modelling to transition metal borides, in order to characterise their structure, stability, and mechanical properties. The obtained trends are used for deciding on perspective systems (e.g., the Ti-W-B system) for further experimental validation and application-orientated coating development.

MM 42.4 Wed 13:00 BAR 205

Atom-mining: Improving the spatial resolution of Field Ion Microscopy using atomistic simulations and data mining — •Gh Ali Nematollahi[1], Shyam S. Katnagallu[1], Michal Dagan[2], Baptiste Gault[1], Blazej Grabowski[1], Paul Bagot[2], Michael Moody[2], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany — [2]Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH UK

Field Ion Microscopy (FIM) relies on the ionization of inert gas atoms from the specimen surface subjected to an intense electric field. Any FIM image represents a "snapshot" of individual surface atoms and 3D information of the bulk can be obtained by removing the surface atoms using field evaporation. However, the analysis of the atomistic information is not straightforward due to strong deformations and intensity variations caused by the electric field, and so far automated techniques to reconstruct the 3D atomistic structure are lacking. In this work, building on recent efforts by Dagan et al.[Microsc. Microanal.], we developed a new framework for automated reconstruction, using data mining and atomistic simulation techniques. In particular, different unsupervised and semi-supervised machine learning techniques are used to detect atoms, crystallographic planes and defects in FIM image. The results show that machine learning can be successfully employed to correct for the deformation of the sample caused by the strong electric fields. In a last step, atomistic relaxation based on empirical potentials is used to further improve the 3D-reconstructed data.