MM 25: Data Driven Materials Science: Computational Frameworks / Chemical Complexity

Time: Wednesday 15:45–18:30 Location: H46

Topical Talk MM 25.1 Wed 15:45 H46

Automated atomistic calculation of thermodynamic and thermophysical data — •Jan Janssen[1,2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Los Alamos National Laboratory, Los Alamos, USA — [3]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

A major challenge in predicting the properties of materials at realistic conditions is the accurate inclusion of finite temperature effects. Doing this on an ab initio level often requires complex simulation protocols. These complex protocols, which often couple several specialized codes, make a quantitative description of error propagation and uncertainty quantification a critical issue.

To handle this high level of complexity we have developed an integrated development environment (IDE) called pyiron - http://pyiron.org. pyiron has been specifically designed to scale simulation protocols from the interactive prototyping level up to the high throughput level, all within the same software framework.

We highlight two recent success stories towards automated calculation of phase diagrams: We first discuss with the automated convergence for all key parameters in DFT codes, followed by the calculation of melting points with a guaranteed precision of better than 1K. These fully automated high-precision tools allow us to study trends over the periodic table in an efficient and systematic way. Examples how such high-throughput screenings allow to develop new strategies in designing materials will be given.

MM 25.2 Wed 16:15 H46

Efficient parameterization of the atomic cluster expansion — •Anton Bochkarev, Yury Lysogorskiy, Matous Mrovec, and Ralf Drautz — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

The atomic cluster expansion (ACE) is a machine learning model with a complete basis set representation that can be used for constructing interatomic potentials. These potentials can be both, general-purpose as well as potentials designed for a specific application. The former are usually more reliable and accurately describe materials in various conditions, but building such models often requires a materials specific expertise and extensive training datasets. Purpose-specific potentials have only limited ranges of applicability, but are also less demanding in terms of training data. Here we demonstrate a complete, efficient and largely automated framework for constructing quantum accurate ACE models for various applications. Our framework includes automated data generation, model parameterization and validation. Efficient implementations on CPU and GPU hardware enable large scale simulations.

MM 25.3 Wed 16:30 H46

Atomic cluster expansion for Mg: From defects to phase diagrams — •Eslam Ibrahim, Yury Lysogorskiy, Matous Mrovec, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, 44780 Bochum, Germany

In this work, we developed a general-purpose parametrization of the atomic cluster expansion (ACE) for Mg. The model shows an outstanding transferability over a broad range of atomic environments and is able to capture physical properties of bulk as well as defective Mg phases in excellent agreement with reference first-principles calculations. We demonstrate the computational efficiency and the predictive power of ACE by calculating the phase diagram covering temperatures up to 3000 K and pressures up to 80 GPa using state-the-art thermodynamic integration techniques implemented in the CALPHY software package. The ACE predictions are compared with those of common interatomic potentials, such as the embedded atom method or the angular-dependent potential, as well as a recently developed neural network potential. The comparison reveals that ACE is the only model that is able to predict both qualitatively and quantitatively correctly the phase diagram in close experiment with experimental observations.

MM 25.4 Wed 16:45 H46

Learning design rules for selective oxidation catalysts from high-throughput experimentation and artificial intelligence — •Lucas Foppa[1], Christopher Sutton[1], Luca M. Ghiringhelli[1], Sandip De[2], Patricia Löser[3], Stephan Schunk[2,3], Ansgar Schäfer[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Germany — [2]BASF SE, Germany — [3]hte GmbH, Germany

The design of heterogeneous catalysts is challenged by the complexity of materials and processes that govern reactivity and by the very small number of good catalysts. Here, we show how the subgroup-discovery (SGD) artificial-intelligence *local* approach[1] can be applied to an experimental plus theoretical data set to identify constraints or *rules* on key physicochemical parameters that exclusively describe materials and reaction conditions with outstanding catalytic performance.[2] By using high-throughput experimentation, 120 SiO_2-supported catalysts containing Ru, W and P were synthesized and tested in propylene oxidation. As candidate descriptive parameters, the temperature and ten calculated parameters related to the composition and chemical nature of elements in the catalyst materials, were offered. The temperature, the P content, and the composition-weighted electronegativity are identified as key parameters describing high yields of value-added oxygenate products. The SG rules reflect the underlying processes associated to high performance, and guide catalyst design.

[1] B.R. Goldsmith, *et al.*, *New. J. Phys.* **19**, 013031 (2017).
[2] L. Foppa, *et al.*, ACS Catal. 12, 2223 (2022).

15 min. break

Topical Talk MM 25.5 Wed 17:15 H46

Understanding Dislocation Flow and Avalanches in High Entropy Alloys by Machine Learning-based Data Mining of In-Situ TEM Experiments — •Stefan Sandfeld — FZJ/IAS-9, 52068 Aachen, Dennewartsstr. 25-27

This talk will give an overview over recent developments in the field of material informatics and materials data science, in particular over current, state-of-the-art machine learning and data-mining techniques in the context of TEM experiments.

As a main example, the goal is to understand some of the many open questions concerning the underlying structure-property relations in High Entropy Alloys (HEAs). Although in-situ Transmission Electron Microscopy (TEM) allows high-resolution studies of the structure and dynamics of moving dislocations and – in a way – makes the local obstacle/energy "landscape" visible through the geometry of dislocations; a 3D analysis and high-throughput data-mining of the resulting data is still not possible.

We introduce a novel data-mining approach that is based on spatio-temporal coarse graining of TEM dislocation data, making ensemble averaging of a large number of snapshots in time possible. Using dislocations as "probes" we investigate the effect of pinning points on the dislocation glide behavior of CoCrFeMnNi alloy during in-situ TEM straining. Additionally, we use our Deep Learning-based dislocation extraction and 3D reconstruction to analyze the strain avalanche statistics of in-situ TEM recordings and discuss the dependency of the power law exponent based on 3D dislocation dynamics simulations.

MM 25.6 Wed 17:45 H46

Phase stability and short range order in CrCoNi medium entropy alloy — •Sheuly Ghosh[1], Vadim Sotskov[2], Alexander Shapeev[2], Fritz Koermann[1,3], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]Skolkovo Institute of Science and Technology — [3]Delft University of Technology

One of the key components in the design and exploration of multi-component alloys is the knowledge about its phase stability. The solid solution of multicomponent alloys are often assumed to be ideally random. However, short-range order, which is challenging to quantify by experiments, is known to affect the mechanical properties of alloys. An important issue to address is therefore to quantify the degree of local chemical ordering as function of temperature and its chemical nature.

In the present work, we have investigated short-range order (SRO) and its impact on phase stability in CrCoNi medium entropy alloy. This alloy is known for its cryogenic damage tolerance and general mechanical superiority. For this purpose, we have employed a recently proposed computationally efficient on-lattice machine-learning interatomic potential called low-rank potentials. These potentials are capable of accurately representing interactions in a system with many

chemical components which is used in subsequent Monte Carlo simulations. The potentials are trained on DFT supercell calculations and thus allow to systematically include the impact of local lattice distortions. The computed short-range order parameters and observed ordering are discussed in view of recent simulation and experimental works.

MM 25.7 Wed 18:00 H46

Inverse Design of Multicomponent Crystalline Materials — Teng Long[1,2] and •Hongbin Zhang[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany — [2]School of Materials Science and Engineering, Shandong University, Jinan 250061, China

Autonomous materials discovery with desired properties is one of the ultimate goals of materials science. In this work, we implemente and apply constrained crystal deep convolutional generative adversarial networks to design unreported (meta-)stable crystal structures. The essential continuous latent space is obtained based on the voxel construction of crystal structures, resulting in an image-based latent space which is proven to be a robust descriptor for forward inference of various physical properties. This also allows prediction of new crystal structures based on generative adversarial network. Furthermore, taking the formation energy as an example, it is demonstrated how the physical properties can be optimized automatically in the latent space while exploring a big chemical space to predict novel phases. Such an approach has been successfully applied on binary (e.g., Bi-Se) and multicomponent systems, which paves the way to achieve the inverse design of crystalline materials via multi-objective optimization.

MM 25.8 Wed 18:15 H46

Databases for Machine Learning of Grain Boundary Segregation — •Alexander Reichmann[1], Christoph Dösinger[1], Daniel Scheiber[2], Oleg Peil[2], Vsevolod Razumovskiy[2], and Lorenz Romaner[1] — [1]Department of Materials Science, Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria

The chemical and structural state of grain boundaries (GBs) is of great importance for the design and performance of many technologically relevant materials. On the basis of atomistic simulations, the relevant quantities of GB, in particular the segregation energy has been calculated for many materials. On the experimental side, the concentration of solute elements at the GBs can be measured with a variety of techniques including in particular Auger spectroscopy or Atom Probe Tomography. When comparing calculated segregation energies with segregation energy gained from experimental excess data, good agreement is not always observed. In this talk we will present our current and planned activities regarding creation of segregation databases and application of data driven models. One of these is the Bayesian inference framework, which we used in combination with Markov chain Monte Carlo simulations for uncertainty quantification and model evaluation. These activities shall lead to a better understanding of the deviation between DFT-calculated and experimentally determined GB excess.