MM 37: Topical session: Data driven materials design - defect engineering

Time: Wednesday 10:15–11:45 Location: BAR 205

Topical Talk MM 37.1 Wed 10:15 BAR 205

Data-driven theory-guided materials design containing scale-bridging concepts — •Martin Friák[1,2,3], Stefanie Sandlöbes[4,3], Zongrui Pei[3], David Holec[5], Mojmír Šob[2,1,6], Jörg Neugebauer[3], and Dierk Raabe[3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [4]Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany — [5]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Ab initio based calculations combined with scale-bridging models have recently emerged as powerful tools in modern materials design. Their further enormous progress has just started thanks to the recent onset of open-access databases with quantum-mechanical results. The talk will provide selected examples of materials development based on data-driven analysis, its combination with traditional concepts (e.g., CALPHAD) and experimental verification. The theory-guided materials design will be exemplified by the case of novel ductile Mg-based alloys assessed by pattern extraction, introduction of generalized descriptors, and multi-dimensional search for optimum compositions. Further, the development of new superalloys employing open-access databases will illustrate the need of their critical cross-validation against experiments.

MM 37.2 Wed 10:45 BAR 205

SEGROcalc, a computational toolbox and database for grain-boundary engineering — Daniel Scheiber, Anatol Drlicek, Nada Kulo, Jürgen Spitaler, Vsevolod Razumovskiy, and •Lorenz Romaner — Materials Center Leoben Forschung GmbH, Roseggerstasse 12, 8700 Leoben, Austria

Segregation of solute elements to grain boundaries (GBs) is a key factor affecting production and performance of many technologically relevant materials. It influences fundamental material properties such as formability, crack propagation, grain growth, precipitation, diffusivity or electric conductivity. By controlling the segregation state, a lever for developing materials of superior properties can be obtained. In this talk we present the development of SEGROcalc, a software for inspecting segregation at GBs and estimating the impact of segregation on materials properties. The basis for the software is formed by a database where a vast amount of literature values of segregation energies and strengthening energies are collected together with the necessary metadata providing information about material, GB structure, segregation site, literature source, or method. The method includes density functional theory calculations, phenomenological modeling and experimental data. The database is accessible via a graphical user interface which allows analyzing the database entries, monitor GB structure, compare segregation energies from different sources, identify solutes beneficial for GB strength and estimate chemical composition of the GB. Representative examples will be shown and the current level of agreement between different theoretical models and experiment discussed.

MM 37.3 Wed 11:00 BAR 205

Efficient sampling in materials simulation - Exploring the parameter space of grain boundaries — Josua Gösmann[1], Christian Greiff[1], Holger Dette[1], and •Rebecca Janisch[2] — [1]Department of Mathematics, Institute of Statistics, Ruhr-Universität Bochum, Germany — [2]ICAMS, Ruhr Universität Bochum, Germany

High-throughput numerical simulations as well as experiments allow a systematic variation of individual parameters, such as e.g.composition, and the coverage of a broad range of these parameters. Nevertheless, the majority of properties that are available today are so-called intrinsic properties like stability, stiffness, or band gaps. Extrinsic properties, like interface distribution functions, energies or mobilities, are less frequently available. As a matter of fact, because they depend on several variables at the same time, such properties form multidimensional databases of their own for one particular material. For such cases we want to promote an efficient sampling of the variable space that is based on design of experiment principles. As a suitable example we pick grain boundary energies, which depend on five geometric degrees of freedom.

We introduce two methods to improve the current state of the art. Based on an existing energy model the location and number of the energy minima along which the hierarchical sampling takes place is predicted from existing data points without any a-priori knowledge, using a predictor function. Furthermore we show that in many cases it is more efficient to use the above mentioned sequential sampling, rather than sampling all observations homogeneously in one batch.

MM 37.4 Wed 11:15 BAR 205

Environmental tight-binding modelling of structural defects in metals — •Eunan J. McEniry, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The modelling of structural defects in metallic systems, such as phase boundaries and dislocations, involves a complex interplay between the chemical composition and the local atomic coordination. Specific challenges include the role of incoherency, the preferential segregation of light elements such as carbon and hydrogen to such defects, and the need to efficiently describe the interactions of compositionally complex systems. While the chemical complexity can be described accurately within density functional theory approaches, the computational cost becomes prohibitive when studying, for example, hydrogen segregation to incoherent phase boundaries between a host matrix and a precipitate.

The environmental tight-binding approach offers a rigorous and computationally efficient framework in which high-throughput atomistic simulations of multi-component systems can be performed, which retains the full quantum-mechanical nature of the problem. The development of potentials derived from this approach will be illustrated, demonstrating the flexibility and speed of the method. As an example, the energetics and diffusion behaviour of hydrogen at the incoherent phase boundary between α-Fe and TiN will be presented.

MM 37.5 Wed 11:30 BAR 205

The shear instability energy as a new parameter to characterise deformation behaviour of materials — Mansour Kanani[1], Alexander Hartmaier[2], and •Rebecca Janisch[2] — [1]School of Mechanical Engineering, Shiraz University, Iran — [2]ICAMS, Ruhr-Universität Bochum, Germany

Systematic relationships between a limited number of fundamental material properties and the observable behaviour of a material are needed for successful design of new materials. To this purpose we introduce the shear instability energy Γ as a new materials parameter. Using interfaces in lamellar TiAl as a case study, we show that Γ can link stacking fault energies from a quasistatic (e.g. ab initio density functional theory based) calculation with the deformation mechanisms that are observed in a molecular dynamics simulation of shear.

Furthermore the shear instability energy can be used to scale between the results of calculations with different interatomic potentials, i.e. also to evaluate trends in deformation mechanisms across different elements. In this, the concept of the shear instability energy is more comprehensive than models which rely only on the ratio of unstable and stable stacking fault energies. This makes it a promising tool for enhancing high-throughput characterization of materials.