# MM 21: Topical Session Electron Theory I

Time: Wednesday 11:00–13:00 Location: IFW A

**Topical Talk** MM 21.1 Wed 11:00 IFW A

**Materials design based on ab initio thermodynamics: Development of accurate and efficient multiscale strategies** — •Jörg Neugebauer, Blazej Grabowski, Fritz Körmann, Martin Friak, and Tilmann Hickel — Max-Planck-Institut für Eisenforschung, Düsseldorf

The combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts has quickly advanced in the past few years and allows now to tackle even complex engineering systems such as polycrystals or steels. Key to these studies is the highly accurate determination of free energies and surfaces. In the first part of the talk it will be shown how efficient sampling strategies together with high convergence density-functional theory calculations allow an accurate determination of all relevant temperature dependent free energy contributions such as electronic, harmonic, anharmonic, magnetic and structural excitations. Using these results to construct coarse grained models stability issues and mechanical properties of various alloys have been computed. The flexibility and the predictive power of this approach will be discussed in the second part of the talk for a few examples: Martensitic transitions in magnetic shape memory alloys, the design of novel light weight alloys, failure mechanisms in novel steels and unraveling design principles in biological structural materials.

**Topical Talk** MM 21.2 Wed 11:30 IFW A

**Diffuse scattering methods as a testbed for alloy theory** — •Harald Reichert — European Synchrotron Radiation Facility, 38043 Grenoble, France

Based on high energy x-ray scattering we have developed new experimental tools in order to reveal details in the energetics of binary alloys with very high accuracy. The technique allows to collect scattering patterns in planes or, more recently, in 3D volumes in reciprocal space. High energy X-ray scattering is characterized by a large Ewald sphere. Similar to transmission electron microscopy, it is possible to map entire planes in reciprocal space with a single exposure employing 2D detectors. In the time-resolved mode the technique allows to follow phase transformations in-situ. In parallel, we have combined first-principles calculations of the alloy energetics with reciprocal space methods for the interpretation of the experimentally determined diffuse scattering maps. This has allowed us to separate chemical and strain-induced components in the effective pair interactions and visualize competing interactions in binary alloys. Applications of this general scheme to a number of binary metallic alloy systems will presented.

**Topical Talk** MM 21.3 Wed 12:00 IFW A

**From electronic structure to real materials properties: Concepts and realization** — •Stefan Müller — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

Due to their predictive power, methods based on electronic structure theory are more and more applied for modelling real materials properties within a quantum mechanical framework. From a technical point of view, the vision behind is the design of functional materials with special properties before expensive experiments are performed. For this, the combination of different methods is a must to describe materials' behaviour from the atom up to the microstructure. In this contribution, recent developments, possibilities and limitations to study real materials properties by first-principles methods will be discussed. It will be shown that the application of an atomistic approach to materials allows for the quantitative description of properties, e.g. ordering parameters and phase boundaries, defects and dislocation behaviour, compressibility and elastic constants or piezo-response tensors and dielectric constants. Regarding systems, the examples reach from metal alloys and adsorption systems to niobates and hybrid materials.

MM 21.4 Wed 12:30 IFW A

**Atomistic modelling of interfaces between cubic phases and topologically close-packed phases in refractory metals** — •Thomas Hammerschmidt[1], Bernhard Seiser[2], Miroslav Cak[1], Ralf Drautz[1], and David G. Pettifor[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]MML, University of Oxford, United Kingdom

The formation of topologically close-packed (tcp) phases in Ni-based superalloys leads to the degradation of the mechanical properties and is attributed to high local concentrations of refractory elements. It is well known that the structural stability of these phases is driven by the average d-band filling. We demonstrate that this structural trend can be understood with a canonical d-band tight-binding model by comparing to our extensive density-functional theory calculations for tcp phases. In order to understand the precipitation of tcp phases, we investigate the structure and energetics of interfaces between the cubic phases bcc and fcc and the topologically close-packed phases $\sigma$ and A15. In particular, we employ analytic bond-order potentials (BOPs) that provide an approximation to the tight-binding model and are suitable for large-scale atomistic simulations. We demonstrate the applicability of recently parametrised BOPs for refractory elements to the description of tcp phases at elevated temperatures and report on the first dynamic simulations of interfaces between cubic phases and topologically close-packed phases.

MM 21.5 Wed 12:45 IFW A

**Tight-binding simulation of complex metallic alloys** — •Eunan J. McEniry, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Stiepeler Strasse 129, 44801 Bochum, Germany

The interplay between various co-existing phases of metallic alloys is a key factor in the determination of the strength, ductile and magnetic properties of modern steels. While ab-initio density-functional theory provides an accurate description of the electronic and mechanical properties of metallic systems, the methodology is prohibitively expensive when applied to larger multi-component systems. While empirical interatomic potentials can be applied to such systems, there are significant question marks over the transferability of these models when applied to systems to which they have not been fitted. The tight-binding approach lies in an intermediate region, enabling the simulation of several thousands of atoms, while retaining the essential physics of bonding and cohesion in solids,

The aim of the present work is to produce a systematic approach which is generally applicable to the full block of transition metals, and which can be applied directly within existing scale-bridging methodologies. We have therefore developed a general tight-binding approach for the simulation of complex metallic alloys, in which the parameterisation is obtained directly from ab-initio calculations. In order to assess the quality and transferability of the approach, we have extensively applied the resulting models to a wide range of alloy structures.