

## MM 13: Computational Materials Modelling III - Alloys

Time: Monday 15:45–17:00

Location: TC 006

MM 13.1 Mon 15:45 TC 006

**Cluster expansions for kinetic Monte-Carlo simulations: towards time evolution with DFT accuracy** — •TOBIAS C. KERSCHER<sup>1,2</sup>, MARTIN LEITNER<sup>1</sup>, STEFAN MÜLLER<sup>2</sup>, and RAIMUND PODLOUCKY<sup>1</sup> — <sup>1</sup>University of Vienna, Institute of Physical Chemistry, Vienna, Austria — <sup>2</sup>Hamburg University of Technology, Institute of Advanced Ceramics, Hamburg, Germany

We take first steps towards vacancy-mediated diffusion kinetics in aluminum alloys (e.g., Ni–Al and Fe–Al) by the combination of an ab initio based cluster expansion (CE) with Monte-Carlo simulations (MC). This method will incorporate many-body effects as well as variable transition barriers that depend on the structural environment of the jump, which is paramount for the calculation of MC jump rates according to transition state theory.

First, we present the energetics of selected transition paths in those Al alloys, determined by density functional theory (DFT) and the nudged-elastic-band method (NEB). Then, we show how the UNCLE code [1] and its kinetic Monte-Carlo algorithm will use a CE framework to include not only the energetics of all possible initial and final configurations of a transition, but also the correct configuration-dependent saddle points of the corresponding transition paths. Both contributions will be separately modeled by CEs based on ab initio input from DFT: the former by the energies of fully-relaxed input structures, the latter by the saddle points of the NEB method.

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[1] D. Lerch *et al.*, Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

MM 13.2 Mon 16:00 TC 006

**Tight-binding modelling of complex alloys: methods and challenges** — •EUNAN J. MCENIRY, GEORG K. H. MADSEN, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, Stiepelers Strasse 129, 44801 Bochum, Germany

In order to reliably model the effects of both alloying and light elements within steels, it is essential to properly take into account the chemistry of the bonding between atoms, as well as the effects of charge transfer and magnetism. Density-functional theory provides such a reliable framework, but its computational expense places limitations on its applicability to large-scale and/or multi-component systems. The tight-binding approximation, including charge transfer and magnetism, can be derived directly from the Kohn-Sham energy functional. Since the electronic structure is obtained from a parametrised tight-binding Hamiltonian, the methodology offers an enormous computational advantage over ab-initio methods.

While many tight-binding models have obtained their parameters from density-functional calculations, they generally involve uncontrolled approximations for the matrix elements of the Slater-Koster Hamiltonian, which limits their transferability. The present work begins with the Harris-Foulkes energy functional, from which the parameters of the tight-binding model are obtained in a rigorous and unambiguous manner. We obtain transferable parametrisations of the environmental contribution to the tight-binding Hamiltonian and assess the validity of the approach by application to nickel-cobalt alloys.

MM 13.3 Mon 16:15 TC 006

**Theoretical investigation of Cr-Sb compounds - structure and magnetic properties** — •G. KUHN<sup>1</sup>, S. MANKOVSKY<sup>1</sup>, S. POLESYA<sup>1</sup>, H. EBERT<sup>1</sup>, M. REGUS<sup>2</sup>, and W. BENSCH<sup>2</sup> — <sup>1</sup>Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany — <sup>2</sup>Christian-Albrechts-Universität, Insti-

tut für Anorganische Chemie, Max-Eyth-Straße 2, 24118 Kiel, Germany

We present a theoretical investigation of structural and magnetic properties of Cr-Sb compounds on the basis of ab-initio electronic structure calculations using the KKR Green's function method. Various compounds with different Cr:Sb ratio have been considered: Cr<sub>3</sub>Sb in  $\beta$ -tungsten-structure, CrSb in NiAs-, NaCl-, Wurtzite- and Zinkblende-structure and CrSb<sub>2</sub> in marcasite- and CuAl<sub>2</sub>-structure.

The structural and magnetic stability have been analyzed performing total energy calculations. Magnetic properties of Cr-Sb compounds have been studied via Monte Carlo simulations based on the Heisenberg model with the exchange coupling parameters obtained by electronic structure calculations using the so-called Lichtenstein formula. This gives us both, the ground state magnetic structure of the compounds as well as their critical temperature which are found in rather good agreement with the experiment.

MM 13.4 Mon 16:30 TC 006

**Effects of In concentration in CuGa<sub>1-x</sub>In<sub>x</sub>Se<sub>2</sub>: a first-principles study** — •ROLANDO SANIZ, DIRK LAMOEN, and BART PARTOENS — Universiteit Antwerpen, Antwerpen, Belgium

Compounds of the family of CuGa<sub>1-x</sub>In<sub>x</sub>Se<sub>2</sub> alloys are of great current interest for the development of better absorbers for photovoltaic applications. To advance our understanding of the effects of alloying ratio,  $x$ , we carried out a state-of-the-art hybrid functional study of the structural and electronic properties of these materials for a series of  $x$  values. In contrast to previous theoretical results, we find that (i) the structural changes induced by increasing In content do not comply to Vegard's law, resulting in fact in a lowering of the symmetry of the system for intermediate In concentrations; (ii) as a function of  $x$ , the fundamental band gap does not follow a quadratic curve defined by a simple “bowing parameter”; (iii) the mixing enthalpies are very low and do not suggest any significant phase separation at finite temperatures.

MM 13.5 Mon 16:45 TC 006

**Ground-state structures and elastic properties of Ni-Ti-Hf shape memory alloys: An ab-initio study** — •JÜRGEN SPITALER<sup>1,2</sup>, DANIEL LÜFTNER<sup>1,2</sup>, ROSTAM GOLESORKHTABAR<sup>1,2</sup>, PETER PUSCHNIG<sup>2</sup>, and CLAUDIA AMBROSCH-DRAXL<sup>2</sup> — <sup>1</sup>Materials Center Leoben Forschung GmbH, Rosegger-Strasse 12, 8700 Leoben — <sup>2</sup>Chair of Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben

Ni-Ti-Hf is a promising shape-memory alloy due to its higher Martensitic transformation temperature as compared to pure NiTi. In this transformation, the energetics and elastic behavior of different crystallographic phases play a crucial role. We have determined the stable phases of NiTi<sub>1-x</sub>Hf<sub>x</sub> in the monoclinic structure (B19') as a function of the Hf concentration using the recently developed ATAT@WIEN2k interface. In order to improve the description of the disordered state, which is crucial for the quality of the expansion, special quasirandom structures were taken into account. We have determined the effective cluster interactions, based on the total energies of the fully-relaxed monoclinic supercells, which yields ordered groundstates for several Hf concentrations. The cluster expansion involves a rather high number of structures with positive formation energies, and it shows that Ti and Hf tend to form layers inside the unit cell. For the obtained groundstates we have determined the full elastic tensors and averaged macroscopic elastic properties structures applying ElaStic, a tool developed in our group.