MM 15: Computational Materials Modelling IV

Time: Tuesday 11:00–13:00 Location: IFW B

MM 15.1 Tue 11:00 IFW B

Atomistic Multi-Time-Scale Modelling of Cu-alloyed α-Fe — •David Molnar[1,2], Peter Binkele[1], Stephen Hocker[1], and Siegfried Schmauder[1,2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart — [2]Stuttgart Research Centre for Simulation Technology (SRC SimTech), SimTech Cluster of Excellence, University of Stuttgart

Cu-alloyed α-Fe changes its material behaviour during its ageing process, especially when operated at higher temperatures of above 300°C, due to Cu-precipitates forming on a relatively large time scale within the Fe-matrix. In order to model this complex behaviour, the growth process of precipitates is accounted for by a Kinetic Monte-Carlo (KMC) approach. Several different precipitation states are transferred from KMC as starting configurations to Molecular Dynamics (MD) simulations allowing for nano tensile tests at different stages of the precipitation process and hence at relevant precipitation times. This can be understood as a multi-time-scale approach in a sequential way. Focusing onto single crystals to reveal the sole effect of the precipitates on the mechanical material behaviour, different structural orientations of the α-Fe matrix are investigated in order to obtain an anisotropic temporal behaviour of, e.g., Young's modulus. Thus, the combination of the methods bridges the short time scale of MD with the longer time scale accessible with KMC simulations. In this way, a computational modelling of tensile tests throughout an ageing process of Cu-alloyed α-Fe is achieved as a step towards multiscale-simulation-based design of materials with desired properties.

MM 15.2 Tue 11:15 IFW B

A mesoscale kinetic model for alloys from atomic Monte Carlo simulations — •Thomas Garnier and Maylise Nastar — CEA, Saclay, France

Atomic Kinetic Monte Carlo (AKMC) simulations allow accurate reproduction of diffusion controlled phenomena in alloys when a rigid lattice can be assumed. However, their computational cost limits their scope. On the other hand, if the efficiency of mesoscopic methods like the Phase field method is not in question, their quantitative predictive power is not ensured most of the time. Some progress in improving the accuracy has been recently reported [1]. Following the same procedure [1], we performed Atomic Monte Carlo simulations and measured the composition fluctuation spectrum to determine mesoscopic energy parameters. To take into account the mesh resolution some finite size effects have to be considered. Another usual weakness of the phase field method is the description of the mobilities. AKMC simulations can once again be exploited to obtain the phenomenological transport coefficients associated with a vacancy diffusion mechanism. The resulting energy and kinetic parameters are then used to parameterize a Cellular Monte Carlo method, which is based on a coarse grained description of the alloy. We demonstrate that such an algorithm allows to obtain consistent results for a grid where each point represents from a few to thousands of atoms. Both thermodynamic and kinetic properties remain almost unchanged with the change of scale.

[1] Q. Bronchart & al, Phys. Rev. Lett.,100,015702,(2008)

MM 15.3 Tue 11:30 IFW B

Polyhedron analysis in complex phases — Thomas Schablitzki, •Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The formation of complex phases in metal alloys can significantly influence the macroscopic properties of the material. Topologically close-packed (TCP) phases in Ni-based superalloys, e.g., are brittle and their formation depletes the matrix of refractory elements which leads to a degradation of mechanical properties. The precipitation of Laves phases in steels, on the other hand, improves the strength of the material through precipitation hardening, whereas the formation of σ-phase precipitates has negative effects.

The atomic structure of complex phases is described by an ordered arrangement of coordination polyhedra around inequivalent lattice sites. To identify the corresponding TCP phases during atomistic simulations we have developed a polyhedron analysis. Of particular importance in trying to understand the formation and growth of TCP phases on an atomistic level are processes taking place at the interface between the complex phase and the alloy matrix. Here, we employ an adaptive kinetic Monte Carlo approach together with our polyhedron analysis to investigate concerted atomic rearrangements at the interface.

MM 15.4 Tue 11:45 IFW B

Structure and energetics of nanoclusters in bcc-Fe containing copper, nickel and vacancies — •Ahmed Tamer Al-Motasem[1], Matthias Posselt[2], Frank Bergner[1], and Uwe Birkenheuer[1] — [1]Institute of safety research — [2]Institute of Ion Beam and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

Reactor pressure vessel (RPV) steels consist of polycrystalline bcc-Fe containing Cu, Ni and other foreign atoms. The continuous irradiation by fast neutrons leads to supersaturation of vacancies and self-interstitials and enhances the diffusion of Cu and Ni which occurs via the vacancy mechanism. These processes favor the formation of nanoclusters consisting of vacancies, Cu and Ni. The interaction of dislocations with these precipitates is considered to be the main cause of hardening and embrittlement of the RPV steels. In order to model the evolution of the precipitates under irradiation by rate theory, the energetics and thermodynamics of the clusters must be known. These data are hardly obtainable by experiments, however, they can be provided by atomic-level computer simulations. In the present work a combination of on-lattice Monte Carlo simulations and off-lattice Molecular Dynamics calculations is employed to determine structure and energetics of the nanoclusters. The atomistic simulations show that ternary clusters exhibit a shell structure with a core consisting of vacancies followed by a shell of Cu and an outer shell of Ni. Binary vacancy-Cu and Ni-Cu clusters show a similar shell structure, whereas the atomic configuration of vacancy-Ni agglomerates is completely different.

MM 15.5 Tue 12:00 IFW B

Phase Diagrams from ab-initio calculations: Re-W and Fe-B — •Thomas Hammerschmidt, Arthur Bialon, Mauro Palumbo, Suzana G. Fries, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

The CALPHAD (CALculation of PHAse Diagrams) method relies on Gibbs energy databases and is of limited predictive power in cases where only limited experimental data is available for constructing the Gibbs energy databases. This is problematic for, e.g., the calculation of the phase transformation kinetics within phase field simulations that not only require the thermodynamic equilibrium data but also information on metastable phases. Such information is difficult to obtain directly from experiment but ab-initio calculations may supplement experimental databases as they comprise metastable phases and arbitrary chemical compositions. We present simulations for two prototypical systems: Re-W and Fe-B. For both systems we calculate the heat of formation for an extensive set of structures using ab-initio calculations and employ the total energies in CALPHAD in order to determine the corresponding phase diagrams. We account for the configurational entropy within the Bragg-Williams approximation and neglect the phenomenological excess-term that is commonly used in CALPHAD as well as the contribution of phonons and electronic excitations to the free energy. According to our calculations the complex intermetallic phases in Re-W are stabilized by the configurational entropy. For Fe-B, we calculate metastable and stable phase diagrams including recently predicted new stable phases.

MM 15.6 Tue 12:15 IFW B

Atom probe tomography as a tool to determine binding energies in Cu_3Au — •Torben Boll[1,2], Talaat Al-Kassab[1,2], Zhiyong Zhu[1], and Udo Schwingenschlögl[1] — [1]Division of Physical Sciences and Engineering King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Binding energies are important parameters for many material properties. In this paper simulations and experimental results of atom probe tomography data for $L1_2$-Cu_3Au will be presented. An important parameter in the simulations is the binding between the different species. A (12,6)-Lennard-Jones potential is assumed to govern the binding and thus the evaporation process, which is modeled according to the Müller-Schottky theorem. By adjusting the Cu-Au-binding potential

of the simulation to fit the experimental results a very good agreement can be reached.

The conclusion is supported by simulations and experiments for the <220> and <200> crystallographic superstructure and the <111> non-superstructure directions.

For comparison a density functional theory method was applied to determine the binding energies. The findings further support our APT-based approach.

MM 15.7 Tue 12:30 IFW B

Effect of uniaxial loading on the structural anisotropy and the dynamics of atoms of Cu-Zr metallic glasses within the elastic regime studied by molecular dynamic simulation — •Yue Zhang[1], Norbert Mattern[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, D-01062 Dresden, Germany

The changes in the structure and the dynamics of atoms and the stress-induced structural anisotropy of a Cu50Zr50 metallic glass upon the application of uniaxial compressive and tensile stresses within the elastic regime during the loading and unloading processes have been studied using molecular dynamic simulation. It is found that the structural change is more significant under tension than under compression, which is accompanied with the destruction of the full icosahedra clusters into distorted ones. Permanent structural change is found at the applied tensile stress of 1000 MPa but still within the elastic regime. The structural anisotropy increases monotonously with the applied stress, being more pronounced along the loading direction than the other two free directions. The results of the mean square displacement, the non-gaussian parameter and the mobile atom analysis suggest that the dynamics of the atoms is distinctly different under uniaxial stresses above 800 MPa. The permanent change in the structure and structural anisotropy can be correlated with the change in the dynamics of the atoms.

MM 15.8 Tue 12:45 IFW B

Investigations of charge and energy distributions in electron beam induced deposition of tungsten — •Harald O. Jeschke, Carlos Ortiz, and Roser Valentí — Institut für Theoretische Physik, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

We employ Monte Carlo simulations of particle trajectories to study the irradiation of a SiO_2 substrate and a $W_xC_yO_z$ deposit with a 5 keV electron beam. We determine the energy distribution of backscattered electrons which is important for the fragmentation of adsorbed $W(CO)_6$ precursor molecules. We also study the distribution of positive and negative charges in deposit and substrate as function of depth and radial distance from the beam center in a cylindrical geometry. Finally, we determine the profiles of the deposited energy which lead to nonequilibrium electron distributions. We relate our findings to experimental observations.