MM 54: Computational Materials Modelling VIII - Mechanical Properties and Strain

Time: Thursday 15:45–17:15 Location: TC 006

MM 54.1 Thu 15:45 TC 006

Which alloying element can make tungsten ductile: Insight from density-functional theory — •Hong Li[1,2], Lorenz Romaner[2], Claudia Ambrosch-Draxl[2], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahn-Straße 12, A-8700 Leoben, Austria. — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria.

Based on density-functional theory (DFT), the influence of alloying elements on the $\frac{1}{2}\langle 111\rangle$ screw dislocation in tungsten is investigated to find alloying candidates that make tungsten ductile. The interaction between the alloying atom and the dislocation is calculated by varying the distance between the position of the alloying atom and the center of the dislocation. Positions near the dislocation center turned out to be energetically more favorable for alloying elements with a higher occupation of *d*-electrons. When Mn, Fe, Os or Ir is placed outside the inner most dislocation core, the dislocation starts moving towards this alloying atom. Furthermore, the change of dislocation core symmetry via alloying is determined using both DFT and the inter-row potential approach. A transition from a symmetric to an asymmetric core is revealed for Re, Os, and Ir. Our results implicate that these elements have similar effects on the $\frac{1}{2}\langle 111\rangle$ screw dislocation in tungsten, and therefore, provide atomistic insights to the development of new tungsten materials.

MM 54.2 Thu 16:00 TC 006

How do residual stresses influence the mechanical properties of severly plastically deformed metal composites? — •Tom Marr[1], Jens Freudenberger[2], Alexander Kauffmann[1,2], Hansjörg Klauss[2], and Ludwig Schultz[2] — [1]TU Dresden, Dresden, Germany — [2]IFW Dresden, Dresden, Germany

Severe plastic deformation at room temperature or at temperatures below the recrystallization temperature of various materials is often used to enhance their mechanical properties. By applying these techniques, work hardening is achieved which goes along with a strong grain refinement, texture sharpening and changes in grain boundary characteristics. Residual stresses in these materials are another factor that might contribute to the effective mechanical properties. Surprisingly few works are dealing with this issue despite the fact that especially in composite materials residual stresses are likely to be observed when severe deformation is applied.

In this work, CP titanium, an Al alloy 5049 as well as a composite material made from both materials are cold deformed to logarithmic deformation strains of $\eta = 4$. Tensile tests are carried out on each of them, while finite element calculations are used to simulate the deformation regime of the composite. Finally, a suggestion is given on how residual stresses can act as a contribution to mechanical properties of severely plastically deformed materials on top of cold work, grain refinement, texture development and grain boundary characteristics changes.

MM 54.3 Thu 16:15 TC 006

A canonical stability/elasticity relationship verified for 200.000 face-centered cubic structures — •Sascha B. Maisel, Michaela Höfler, and Stefan Müller — Insitute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

By systematic studies of binary alloy systems via density functional theory and the cluster expansion approach we show that the elastic properties of face-centered cubic intermetallics obey certain rules. Firstly, the stiffness and the heat of formation are negatively correlated with a nearly constant Spearman correlation for all concentrations. Secondly, the probability to find a very stiff structure is negligible in the limit of high enthalpy excess. Lastly, we quantify the probability of finding a meta-stable structure σ harder than the ground-state γ at a specific concentration $x(\sigma) = x(\gamma)$ depending on σ's distance to the ground-state line. The consequences are discussed from both a mathmatical and an application-oriented perspective.

MM 54.4 Thu 16:30 TC 006

Role of coherency strain in the stabilization of metastable precipitate of the Mo-C binary system — •Sankari Sampath, Rebecca Janisch, Suzana G Fries, and Alexander Hartmeier — ICAMS, Bochum, Germany

The precipitation of second phases in metals and metallic alloys is an important phenomenon that has a high influence on the mechanical properties of the material. In a previous computational study, the precipitation behavior of (bct)carbide, MoCx at a grain boundary in Mo(bcc) has been investigated. The study showed that there is a significant strain contribution to the interface energy of the lattice misfit. In the present project, the Mo-C binary system is being studied thoroughly by varying carbon concentrations in the system. The aim is to quantify this strain contribution to the interface energy by means of ab-initio Density Functional Theory using VASP code such that the stabilization of the metastable phase(bct) could be carried out.

The structural stability of various phases of the Mo-C system has been analyzed and compared with experimental results where available.The phase diagram has been obtained using Thermo-Calc and the stable phases agree with our predictions at T=0K. A metastable phase(bct), which is not present in the phase diagram, has been observed experimentally by HREM as a semi-coherent precipitate. We assume that it is stabilized by the precipitate interface energy. Starting with the coherent interface for Mo(001) and MoCx(001),the study has been extended to gamma surface calculations that yield possible Burgers vectors for misfit dislocations.

MM 54.5 Thu 16:45 TC 006

Elastic anomalies and short-range order effects for Ag-Pd alloys — •Martin Hoffmann[1,2], Alberto Marmodoro[3], Eero Nurmi[4], Kalevi Kokko[4], Arthur Ernst[2], and Wolfram Hergert[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Seckendorff-Platz 1, D-06120 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik,Weinberg 2, D-06120 Halle, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom — [4]Department of Physics and Astronomy, University of Turku, FIN-20014 Turku, Finland

We investigate the elastic properties of the binary alloy Ag-Pd. From the experiment it is known that the lattice constant of this system shows a deviation from the expected linear behaviour according to the Vegard's rule. This was formerly studied by assuming a totally disordered alloy and thereby using the coherent potential approximation (CPA). However, there are predictions of three ordered phases in this system and we include them in our study via supercell calculations. Due to the treatment of certain sub-lattices with the CPA in the Korringa-Kohn-Rostoker formalism we are able to explore the equilibrium properties even in the concentration range between the long-range order structures. We obtain again various deviations from the linear behaviour. As former studies assumed such changes could be observed in concordance with electronic topological transitions in the Fermi surface topology. Using the novel concept of the multi sublattice non-local CPA we introduce short-range order within the same supercell construction.

MM 54.6 Thu 17:00 TC 006

Study of structural anisotropy in Cu50Zr45Al5 metallic glass under uniaxial loading by molecular dynamics simulations — •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 structural anisotropy in Cu50Zr45Al5 metallic glass under uniaxial loading from zero up to 1200 MPa was studied by molecular dynamics simulations. The anelastic strain is found to be negligibly small below 600 MPa whereas it increases with the simulation time from 600 to 1200 MPa. The degree of structural anisotropy and the atomic structure were characterized using a second order fabric tensor and Voronoi tessellation, respectively. Structural analysis indicates that the anelastic deformation occurs via the destruction of clusters with high geometric symmetry. Comparing with our previous results, the degree of anisotropy in Cu50Zr45Al5 MG is about 20-30% lower than that in Cu-Zr MGs under similar loading conditions. It indicates that the covalent bonding around Al atoms tends to stabilize the local structure against anelastic deformation in Cu50Zr45Al5 metallic glass. Finally, the relation between the anelastic strain and shear transformation zones (STZs) is discussed.