MM 40: Mechanical Properties and Allloy Design

Time: Thursday 15:45–18:30 Location: SCH A 251

MM 40.1 Thu 15:45 SCH A 251

First principles validation of barriers in Ni_3Al — •Adam Fisher[1], Thomas Hudson[1], Huan Wu[2], Tyler London[2], and Peter Brommer[1] — [1]University of Warwick, Coventry, UK — [2]TWI Ltd, Cambridge, UK

Precipitates in Nickel-based superalloys form during heat treatment on a time scale inaccessible to direct Molecular Dynamics simulation, but can be studied using kinetic Monte Carlo (KMC). This requires reliable values for the barrier energies separating distinct configurations over the trajectory of the system. In this study, we validate barriers found with the activation relaxation technique nouveau (ARTn) method in a Ni_3Al using a published potential for the atomic interactions against first-principles methods. In a first step, we confirmed that the ARTn barrier energies agree with those determined with the nudged elastic band (NEB) method. As the number of atoms used in those calculations is too great for direct *ab initio* calculations, we then cut the cell size to 255 atoms, thus controlling finite size effects. We then use the plane-wave density functional theory (DFT) code CASTEP and its inbuilt NEB method in the smaller cells. This provides us with a continuous validation chain from first principles to large-scale KMC and allows us to quantify the errors incurred in simulations of precipitate formation and evolution.

MM 40.2 Thu 16:00 SCH A 251

Ab-initio study of partitioning of transition-metal elements in the γ/γ' microstructure of single-crystal superalloys — •Isabel Pietka[1], Andreas Förner[2], Manuel Köbrich[2], Steffen Neumeier[2], Ralf Drautz[1], and Thomas Hammerschmidt[1] — [1]Ruhr-Universität Bochum, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science & Engineering

The outstanding mechanical properties at high temperatures of Ni- and Co-base superalloys are closely tied to the underlying γ/γ' microstructure. Understanding the preferences of alloying elements for the γ matrix or γ' precipitates helps to develop new alloy compositions. In this work, we investigate the partitioning of the 3d, 4d, and 5d transition metals (TMs) in Ni_3Al and $Co_3(Al,W)$ superalloys. In particular, we determine the preference of the TM elements for the γ or γ' phase by density functional theory calculations. We find clear trends of partitioning across the TM series that are in good agreement with experimental data. Our findings can be rationalized in terms of band filling and atomic size differences by moments analysis from bond order potential theory.

MM 40.3 Thu 16:15 SCH A 251

Towards understanding the yield stress anomaly of Ni_3Al from the energetics of planar defects — •Xiang Xu[1,2], Xi Zhang[2], Andrei Ruban[3,4], Siegfried Schmauder[1], and Blazej Grabowski[2] — [1]Institute for Materials Testing, Materials Science and Strength of Materials, University of Stuttgart, Germany — [2]Institute for Materials Science, University of Stuttgart, Germany — [3]KTH Royal Institute of Technology, Stockholm, Sweden — [4]Materials Center Leoben Forschung GmbH, Leoben, Austria

The yield stress anomaly of $L1_2$ intermetallic compounds, especially Ni_3Al, has been investigated for several decades. It is believed that planar defects, e.g., the complex stacking fault and the antiphase boundaries, play an essential role in the dislocation activities during plastic deformation. However, a thorough temperature dependence of the formation energy of these planar defects is still elusive. Facilitated by the state-of-the-art methodology which acquires different thermal mechanisms, especially the magnetic excitations and the full vibrations, the Gibbs energies of the complex stacking fault and the antiphase boundaries of Ni_3Al were calculated within the ab-initio framework up to the melting temperature. The accurate results obtained here are helpful to scrutinize the available experimentally measured data and provide fruitful insights to understand the mechanism behind the yield stress anomaly as well.

MM 40.4 Thu 16:30 SCH A 251

Observation of in-plane oriented Guinier-Preston zones in Al-Cu — •Johannes Berlin, Tobias Stegmüller, and Ferdinand Haider — Universität Augsburg, Deutschland

Known for a long time, the first metastable precipitates forming in Al-Cu alloys during natural ageing are the so-called Guinier-Preston zones (GPZ), platelets of Cu on {100} planes of only one atomic layer thickness. With the development of aberration corrected (S)TEMs, direct observation and imaging of these platelets was possible, but with the restriction, that only edge view was possible. Using a Cs-probe corrected scanning transmission electron microscopy with HAADF detector (DF-STEM), a single Cu atom in a Al column results in sufficient contrast to the neighbouring columns. In sufficiently thin samples, planar zones then lead to theoretically forbidden reflections of type {110} in the fourier transformed image, since only half of the columns in the GP zone contain a Cu atom. Thus, fourier filtering of such an image with only these forbidden reflections allows to observe GP Zones in a plan-view. The average size, shape and density of the GP-zones was determined for different aging times, and STEM image simulations using the software package DrProbe support this interpretation.

MM 40.5 Thu 16:45 SCH A 251

Dynamical and structural properties of undercooled Cu-Ti melts — •Lucas Kreuzer[1,2], Fan Yang[2], Thomas Hansen[3], Andreas Meyer[2,3], and Winfried Petry[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Institute for Material Physics in Space, German Aerospace Center (DLR), Cologne, Germany — [3]Institute Laue-Langevin (ILL), Grenoble, France

Cu-Ti alloys feature a large, undercooled liquid region and a high glass-forming ability (GFA) and thus, provide the possibility to obtain two component bulk metallic glasses (BMGs). This unusual behavior could be due to the special properties of the liquid Cu-Ti system: a positive excess volume and a negative enthalpy of mixing. However, the relevant atomic mechanisms responsible for such good GFA are still to be explored. Here we discuss the temperature-dependent dynamical and structural properties of Cu-Ti melts, within a compositional range of 24 to 69 at% Ti. Accurate data about viscosity, density, and atomic structure, the Cu-Ti samples was obtained by using have been processed without any container using the electrostatic levitation technique. We found a non-monotonous trend of the viscosity, with the highest values at intermediate Ti contents. Surprisingly, this dynamical trend is not reflected by the macroscopic packing fraction, meaning a high viscosity does not necessarily correlate with a dense packing. However, on the atomic scale, x-ray and neutron diffraction reveal a denser, local packing and a pronounced chemical short-range order. These short-range interactions can explain the high viscosity, while the macroscopic packing fraction is rather governed by long-range interactions.

15 min. break

MM 40.6 Thu 17:15 SCH A 251

Can we measure twinning stress of a high entropy alloy with micromechanics? — •Camila Aguiar Teixeira, Subin Lee, and Christoph Kirchlechner — Institute for Applied Materials, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

CoCrFeMnNi and CoCrNi high entropy alloys (HEAs) have attracted attention due to their mechanical properties. Extensive mechanical twinning is mainly responsible for their outstanding mechanical response under cryogenic temperatures, e.g. increase in ductility and tensile strength. However, at room temperature dislocation slip is dominant and twinning only observed in highly deformed samples. Although both HEAs have been broadly studied, there is still a lack of in-depth understanding of twinning mechanism and stresses required for its activation, which is crucial for advanced HEAs design. In this work, we aim to develop protocols to assess the critical resolved shear stress required for twinning by applying in situ micromechanics. Therefore, two points were addressed within the scope of this work: (i) study the transition from full to partial slip using micropillar compression and (ii) observe deformation twinning by shear stress using micro-shear test. Specific grain orientations were chosen through EBSD analyses, for the micropillar single slip orientation with higher Schmid factor for partial slip and for micro-shear [1 1 2] ND and [-1 1 1] TD orientation. Samples were then micromachined by FIB and tested in situ. Post-mortem analysis included SEM imaging, EBSD and (S)TEM to verify if twinning could be observed. The results provided quantitative insights essential for further understanding of the twinning mechanisms.

MM 40.7 Thu 17:30 SCH A 251

Influence of crystal structure on helium-induced tendril formation in an FeCoCrNiV high-entropy alloy — •Svenja Lohmann[1], Russell Goodall[2], Gregor Hlawacek[1], René Hübner[1], Le Ma[2], and Amy S. Gandy[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]University of Sheffield, UK

High-entropy alloys (HEAs) are a relatively new class of metal alloys composed of several principal elements, usually at (near) equiatomic ratios. Our goal is to understand how such a multicomponent alloy behaves under irradiation. The FeCoCrNiV HEA exhibits both a face-centred cubic (fcc) and a body-centred tetragonal (bct) phase, thus allowing us to specifically study the influence of crystalline structure at very similar chemical composition. We irradiated both phases with a focussed He beam provided by a helium ion microscope (HIM) at temperatures between room temperature and 500°C. The irradiation fluence was varied between 6×10^{17} ions/cm^2 and 1×10^{20} ions/cm^2. High-resolution images of the irradiated areas were taken with the same HIM. Selected irradiated areas were additionally studied by TEM in combination with EDXS. Under irradiation, pores start to be generated in the material with pore sizes differing significantly between the two phases. At higher fluences and above a critical temperature, a tendril structure forms in both phases. We found that the critical temperature depends on the phase and is lower for fcc. TEM images reveal that the tendrils span the whole depth of the irradiated area, and are accompanied by bubbles of various sizes. Scanning TEM-based EDXS of these structures indicates a He-induced change in composition.

MM 40.8 Thu 17:45 SCH A 251

Diffusion and phase stability in a HCP HfScTiZr multicomponent alloy — •Mohan Muralikrishna Garlapati[1], Sandipan Sen[1], Xi Zhang[2], Sankaran S[3], Juliana Schell[4,5], Lukasz Rogal[6], Gerhard Wilde[1], Grabowski B[2], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Muenster, Muenster, Germany — [2]Institute of Materials Science, University of Stuttgart, Stuttgart, Germany — [3]Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Madras, Chennai, India — [4]European Organization for Nuclear Research (CERN), CH-1211 Geneva, Switzerland — [5]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Essen, Germany — [6]Institute of metallurgy and Materials Science, Polish Academy of Sciences, Krakow, Poland

Phase stability and tracer diffusion in a hexagonal close-packed (HCP) HfScTiZr multicomponent alloy are investigated. The microstructure stability is examined by an in-depth electron microscopy characterization of samples subjected to prolonged heat treatments. It is found that the alloy decomposes into two HCP phases with similar lattice constants. The DFT calculations confirm the possibility of the phase decomposition. The minor and major phases are observed to be enriched with Ti and Sc, respectively. Self-diffusion is measured using the 44Ti, 46Sc, and 89Zr radioactive isotopes. The phase decomposition is found to influence marginally Zr, but significantly Ti and Sc diffusion. The diffusion properties are analyzed in correlation to the microstructure stability and thermodynamic properties of the alloy.

MM 40.9 Thu 18:00 SCH A 251

Solid solution strengthening in single-phase HEAs based on Au-Cu-Ni-Pd-Pt — •Sophie Drescher[1], Jens Freudenberger[1], Sascha Seils[2], Alexander Kauffmann[2], and Martin Heilmaier[2] — [1]Leibniz-IFW Dresden, Helmholtzstr. 20, 01099 Dresden, Germany — [2]Karlsruhe Institute of Technology, Institute for Applied Materials, Engelbert-Arnold-Str. 4, 76131 Karlsruhe, Germany

Solid solution strengthening (SSS) is the dominant strengthening mechanism in High entropy alloys (HEAs). In contrast to dilute alloys,SSS of HEAs is yet not well understood. Therefore, it is necessary to develop reliable models to predict their mechanical properties. To verify such models experimental work is needed that illustrates the concentration-dependent solid solution strengthening of different alloys over a large composition range.

The high entropy alloy system Au-Cu-Ni-Pd-Pt is unique as it crystallizes in face-centered cubic crystal structure and is single-phase presumably within the entire concentration range. Hence, it serves a suitable benchmark system to investigate composition-dependent effects on the strength. In this study, it has been examined whether the model of Varvenne [1] is suitable to predict the SSS in this alloy system. The concentrations of individual elements were varied and the strength and hardness were evaluated. The model of Varvenne is misguiding the development of the strength in a large compositional range. However, the results give insights into the impact of different elements on the strength and can help to further enhance the model.

[1] C. Varvenne, et al., Acta Mater. 118 (2016) 164.

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Magnetism in nanocrystalline CoMnFeNiGa high entropy alloys: "from micro and bulk to nano" — •Natalia Shkodich[1,2], Varatharaja Nallathambi[1,2], Tatyana Smolyarova[1], Sven Reichenberger[1], and Michael Farle[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — [2]Max-Planck-Institut für Eisenforschung Max-Planck-Straße 1, 40237 Düsseldorf, Germany

We report the successful fabrication of three types of CoMnFeNiGa high entropy alloys: a) nanoparticles, b) nanocrystalline micron-sized powder, and c) nanocrystalline metallic bulk. Homogeneous micron-sized CoMnFeNiGa HEA powders with a nanocrystalline structure and compositional homogeneity were produced by high energy ball milling (HEBM) for 190 min in Ar at 900/1800 rpm. From these powders we synthesized (a) homogeneous nanocrystalline bulk HEAs by spark plasma sintering (SPS) and (b) HEA nanoparticles - by laser fragmentation in liquids (LFL). The XRD, SEM/EDX, and HR TEM results showed that single fcc phase nanosized grains (˜10 nm) are obtained after 190 min of HEBM. These partially transform into a bcc one after SPS at 1073K, while the LFL leads to the formation of nanoparticles with two morphologies, that is spheres and platelets with fcc, bcc and hexagonal structures. Fast annealing up to 1000K of HEBM and LFL HEA particles leads to significant structural and composition changes and increases the saturation magnetization Ms (300K) from 35.4 to 96.1 Am2/kg, and from 37.3 to 49.7 Am2/kg, respectively. We acknowledge financial support from DFG (CRC/TRR 270, project S01).