MM 16: Structural Materials

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

MM 16.1 Tue 11:00 IFW D

Temperature dependent lattice misfit in Nickel-base superalloys - Simulation and experiment — •Steffen Neumeier and Mathias Göken — Lehrstühl für Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg, Erlangen, Deutschland

Ni-base superalloys are widely used in high temperature applications like jet engines and land-based turbines, because of their excellent high temperature properties. They derive their excellent high temperature strength and creep resistance from the presence of a high volume fraction of Ni_3Al γ' precipitates ($L1_2$ structure), which are embedded coherently within the face centred cubic (A1) γ matrix. The magnitude and sign of the lattice misfit between γ and γ' are important parameters affecting the microstructural evolution and high temperature strength of Ni-base superalloys. Therefore the knowledge of the lattice misfit at application temperature is of great importance. In this study the lattice misfit of several 1^{st}, 2^{nd} and 4^{th} generation Ni-base superalloys in dependence of temperature has been measured by means of HRXRD and compared with lattice misfit simulations based on thermodynamic calculations. The influence of the thermal expansion coefficients and the change in the chemical composition of both γ and γ' due to the γ' dissolution with increasing temperature has been taking into account. The experimentally measured γ and γ' lattice parameters could be reproduced by the simulation and the γ/γ' lattice misfit could be reasonably predicted.

MM 16.2 Tue 11:15 IFW D

Short-range order in Ni-rich Ni-W alloys investigated by synchrotron measurements and first-principles calculations — •Nils Schindzielorz[1], Sascha Maisel[1], Alexey Bosak[2], Harald Reichert[2], and Stefan Müller[1] — [1]Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg — [2]European Synchrotron Radiation Source (ESRF), 6 Rue Jules Horowitz, F-38043 Grenoble

Ni-rich Ni-W alloys show a whole zoo of short-range order phenomena as observed by diffuse X-ray scattering. It will be shown that the quantitative analysis of these patterns can be successfully performed by the combination of X-ray scattering and ab-initio based calculations. For the latter, the combination of density functional theory with the cluster expansion method as realized in the computer code UNCLE and Monte-Carlo simulations is applied. This allows us to predict the short-range order in real and k-space as a function of concentration and temperature. The predicted patters are compared with experimental data. It turns out that the short-range order in Ni-W can only be explained by the simultaneous existence of different structure types, where the D16 compound plays one important role.

MM 16.3 Tue 11:30 IFW D

Energetics of TiAlNb alloys with interstitial carbon — •Dominik Legut[1,2], Juergen Spitaler[1,2], Pasquale Pavone[1,2], and Claudia Ambrosch-Draxl[1] — [1]Atomistic Modelling and Design of Materials, Leoben, Austria — [2]Materials Center Leoben, Leoben, Austria

TiAl based alloys exhibit attractive properties such as low density, high strength at high temperatures, and very good oxidation resistance. However, they are brittle at room temperature. It was recently found that lamellar structures, obtained by alternating the γ and α_2 phase, addition of transitional metal or interstitial elements like carbon increase ductility and creep strength at room temperature.

We perform first-principles calculations based on density-functional theory to study the influence of interstitial carbon on the energetics of both the γ and α_2 phase of the TiAlNb alloy system, where Nb atoms substitute Ti sites. In particular, we determine the heats of formation with respect to the pure TiAl phases, taking into account various configurations for the substitutional Nb sites. In our calculations, the carbon atoms are located on one of two possible interstitial sites.

We consider two different situations. First, Al-rich systems are obtained by replacing Ti atoms with Nb. Second, in Ti-rich systems, the concentration of Ti atoms is kept constant (50%) by moving the Ti atoms replaced by Nb to Al sites. We find that in all cases the energy cost of accommodating carbon is very much affected by the presence of the alloying element Nb.

MM 16.4 Tue 11:45 IFW D

First principles study of elastic properties of eutectic Ti-Fe alloys up to their mechanical stability limits — •Li-Fang Zhu, Martin Friák, Alexey Dick, Alexander Udyansky, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 402 37, Düsseldorf, Germany

Ti-based alloys have been suggested for commercial applications due to their high strength and good corrosion resistance. Motivated by experimental results showing eutectic Fe-Ti alloys decomposing into the FeTi compound with B2 structure and beta-Ti(Fe) alloys with varying Ti concentration (depending on the cooling rate), Ti-Fe alloys covering a broad range of Ti concentrations were studied using density functional theory (DFT) within the generalized gradient approximation (GGA). After examining thermodynamic stability and structural properties, ground-state single crystalline elastic constants have been calculated and homogenized in order to determine experimentally accessible elastic moduli. Employing the quasi-harmonic approximation, temperature dependences of single-crystaline and polycrystalline elasticity parameters have been predicted. Further, by simulating tensile tests along [001], [110] and [111] directions, the theoretical tensile strengths have been determined for both FeTi-B2 and beta-Ti(Fe) phases. In addition, the brittle-fracture crystal separation was simulated for (001), (110) and (111) planes. Searching for a loading mode of materials failure, our FeTi-B2 results show that the theoretical tensile strength is lowest along the [001] direction and that the brittle-fracture crystal separation energy is lowest for the (110) plane.

MM 16.5 Tue 12:00 IFW D

Ultra fast in situ hard X-rays micro-tomography: Application to solidification and hot tearing of alloys or heat treatment of super conductors — •Mario Scheel[1], Marco Di Michiel[1], Luc Salvo[2], Pierre Lhuissier[2], Bastien Mireux[2], Michel Suéry[2], and Christian Scheuerlein[3] — [1]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France — [2]Laboratoire SIMAP - Groupe GPM2, BP 46 Saint Martin d'hères, France — [3]European Organization for Nuclear Research (CERN), TE-MSC, Geneva, Switzerland

Hard X-rays micro-tomography allows getting 3D images with spatial resolution in the micron range in a non-destructive manner. It has been applied now in a wide range of research fields (damage in materials, foams, solidification, etc.). Thanks to the high flux of synchrotron and ultra fast cameras the total time to acquire a scan was considerably reduced. The use of specific devices mounted (furnaces, tensile compression machine) allows performing in situ tomography on various materials. We performed 3D in situ solidification of aluminium-copper alloys at fast cooling rates (between 1 to 10°C/s) and we will show results on the early stage of solidification (morphology of solid phase, kinetics of growth). In addition the formation of porosity and the phase evolution during the reaction heat treatment of superconducting wires has been monitored.

MM 16.6 Tue 12:15 IFW D

Conical slits for depth-resolved stress measurements with high-energy X-rays — •Torben Fischer, Peter Staron, Eike-Henning Eims, Sebastian Frömbgen, Norbert Schell, Martin Müller, and Andreas Schreyer — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Geesthacht, Germany

The use of photons with energies from about 50 keV up to about 150 keV and the resulting large penetration depths enables diffraction measurements in the bulk of the material and, thus, to obtain information e.g. on residual stresses even within larger components. The depth resolution that is required for such measurements can be achieved by the use of a conical slit system in the case of monochromatic radiation. Such a system was tested at the new high-energy material science beamline HEMS of the Helmholtz-Zentrum Geesthacht at the new PETRA III synchrotron at DESY, Hamburg. The samples used for the test were laser beam welded (LBW) steel sheets. The LBW technique is currently still being developed for applications in civil aircraft production and automotive industry for reducing weight and production costs. The LBW introduces residual stresses in the weld and heat affected zone. These stresses can have disadvantageous influence on the service performance of the weld. LBW overlap joints of DC04 steel with a thickness of 2 mm were investigated by this technique and the results were compared with the results of neutron diffraction measurements.

MM 16.7 Tue 12:30 IFW D

***In situ* investigation of friction stir welded AA7449 using high energy SAXS** — •Malte Blankenburg, Torben Fischer, Peter Staron, Luciano Bergmann, Jakob Hilgert, Jorge F. dos Santos, Martin Müller, and Andreas Schreyer — Helmholtz-Zentrum Geesthacht, Institute of Materials Research, Max-Planck-Strasse 1, 21502 Geesthacht, Germany

Friction stir welding (FSW) has in a very short time found a multitude of applications for high-tech applications in the transportation and energy industries. When engineering metallic materials are joined by friction stir welding, thermo-mechanical processes alter the base metal microstructure and properties. This induces the formation of non-equilibrium microstructures in the joint region, which are significantly different from those found in the base material. Such non-equilibrium phases can reduce strength and toughness of the material and are normally compensated by increasing the dimensions or design complexity of integral structures.

The intermediate stages of precipitation or phase transformations in the weld zone during the joining process can only be registered by *in situ* experiments. The transportable FSW system 'FlexiStir' developed at HZG provides the opportunity to perform *in situ* small-angle X-ray scattering (SAXS) experiments during FSW. So far, FlexiStir was used at the HZG high energy synchrotron beamline HARWI II at HASYLAB. As a result, spatial resolved size and volume fraction distributions of precipitates in the heat affected zone during the FSW process were obtained.

MM 16.8 Tue 12:45 IFW D

Light weight metal compounds with ultra-fine grained microstructure — •Tom Marr[1,2], Jens Freudenberger[2], Juliane Scharnweber[1], Carl-Georg Oertel[1], Werner Skrotzki[1], Uwe Siegel[2], Uta Kühn[2], Jürgen Eckert[2], Ulrich Martin[3], and Ludwig Schultz[1,2] — [1]TU Dresden — [2]IFW Dresden — [3]TU Bergakademie Freiberg

Composites of titanium and aluminium have been severely plastically deformed using a repetitive bundling and swaging technique. This process allows to reaching high logarithmic deformation strains. In consequence, an ultra-fine grained microstructure of all phases is observed, resulting in a high specific strength, making this materials suitable for constructive applications. Among these composites, ultimate tensile strengths of around 800 to 900 MPa are reached in combination with a final mass density of 3-4 g/cm^3.