MM 6: Structural Materials

Time: Monday 10:15–11:15 Location: IFW D

MM 6.1 Mon 10:15 IFW D

Ordering and thermodynamic properties of refractory NbMoTaW alloy from first-principles — •Fritz Körmann[1], Andrei V. Ruban[2,3], and Marcel H.F. Sluiter[1] — [1]Materials Science and Engineering, Delft University of Technology, Delft, Netherlands. — [2]Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden. — [3]Materials Center Leoben, Leoben, Austria.

Some refractory high entropy alloys (HEA) exhibit high-temperature mechanical properties that exceed modern Ni-based super alloys. However, little is known about their fundamental physical properties such as, e.g. ground states, degree of chemical ordering at elevated temperatures or thermodynamic properties. We present a combined first-principles and Monte Carlo (MC) study to investigate ordering at elevated temperatures in the prototype BCC HEA NbMoTaW [1]. Chemical interactions have been computed from first-principles by means of the coherent potential approximation in combination with the screened generalized perturbation method. Local relaxations have been considered by explicit super cell calculations. Surprisingly, the NbMoTaW solid-solution at elevated temperatures does not originate from the small magnitude but rather from the highly frustrated long-ranged nature of the chemical interactions. The role of the chemical interactions and ordering on thermodynamic properties is examined in detail [2]. [1] F. Körmann, A.V. Ruban, M.H.F. Sluiter, Materials Research Letters (2016), DOI 0.1080/21663831.2016.1198837 [2] F. Körmann, M.H.F. Sluiter, Entropy 18, 403 (2016).

MM 6.2 Mon 10:30 IFW D

Micromechanical behavior in dependence of the microstructure of nickel-based superalloys — •Robert Lawitzki[1], Jonas Woste[2], Michael Hofmann[3], Christian Krempaszky[2], Di Wang[4], Guido Schmitz[1], and Julia Wagner[1] — [1]Universität Stuttgart, Institut für Materialwissenschaft, 70569 Stuttgart — [2]TU München, Lehrstuhl für Werkstoffkunde und Werkstoffmechanik, 85748 Garching — [3]TU München, FRM II, 85747 Garching — [4]KIT, Institut für Nanotechnologie (INT), 76344 Eggenstein-Leopoldshafen

Nickel-based superalloys have a huge field of applications, particularly in the high-temperature regions of gas turbines. For those applications the reliable knowledge of residual stresses on different length scales is crucial since they affect the material properties strongly. Beside macroscopic stresses, which influence directly the life time of components, intergranular strains should be taken into account as well, since they always superpose the macroscopic stress state. Those type II stresses, which reflect the micromechanical material behavior, are strongly dependent on the microstructure of the samples.

In this contribution, we present results of mechanical in-situ neutron diffraction tests on the two nickel-based superalloys Inconel 718 and Haynes282. Our data show, that the micromechanical behavior and thus the mechanisms of plastic deformation differ for IN718 and Haynes282. The neutron diffraction results will be discussed in detail with respect to the different observed microstructures, which were characterized in detail by means of electron microscopy like SEM and TEM.

MM 6.3 Mon 10:45 IFW D

Microstructural investigation on the Na2SO4 - NH4Cl salt spray tested Alloy 602CA sheets subjected to different surface modification techniques — •Sai Rajeshwari K[1], Gerhard Wilde[2], Vijay K. Vasudevan[3], and Sankaran S[1] — [1]Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, India — [2]Institute of Materials Physics, University of Münster, Germany — [3]Department of Chemical and Materials Science Engineering, University of Cincinnati, USA

Alloy 602CA is a high temperature corrosion resistant nickel base super alloy with high creep strength in carburizing and oxidizing atmosphere. Alloy 602CA contains 5% (by volume) of Cr23C6 precipitates which act as reservoirs for the formation of a protective Cr2O3 coating in the event of high temperature exposure to oxidation or corrosion. Hence, it is extensively used in thermal, petrochemical and power plant equipment. Corrosion due to Na2SO4 salt deposition is a major challenge and involves high cost.An attempt is made to improve the high temperature corrosion resistance and fatigue properties of the Alloy 602CA sheets through two surface modification techniques namely, High Reduction Cold Rolling (HRCR) and Ultrasonic Nanocrystal Surface Modification (UNSM).Microstructural and corrosion behavior investigations employing Scanning Electron Microscopy and Energy Dispersive Spectroscopy of HRCR and UNSM treated alloy 602CA sheet samples subjected to Na2SO4 :NH4Cl (80:20)salt spray tests for varying duration of 20, 40 and 60 hours at 925°C will be discussed in detail.

MM 6.4 Mon 11:00 IFW D

Tungsten fiber reinforced tungsten (Wf / W) produced by CVD and CVI — •Leonard Raumann[1], Jan Willem Coenen[1], Johan Riesch[2], Hanns Gietl[2], and Christian Linsmeier[1] — [1]Institut für Energie und Klimaforschung Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching b. München

Due to excellent thermal and hydrogen retention properties, tungsten is the main candidate for first wall and divertor materials in future fusion reactors. However, the intrinsic brittleness of tungsten is a concern regarding high transient heat loads and neutron irradiation in the fusion environment. To overcome this drawback, tungsten fiber reinforced tungsten (Wf/W) composites are being developed relying on an extrinsic toughing principle. One processing route is the chemical vapor deposition and infiltration of tungsten fiber fabrics. The major challenge for this route is to prevent voids within the composite, which can easily occur if the tungsten film growth separates not yet infiltrated domains from gas flow supply. To achieve fully dense materials the underlying principles have to be fully understood. To asses this process parameters are varied in simplified experimental setups to bring a simulation model in line with the experimental data. The model is taking into account the kinetics for adsorption of the reactants, surface reactions, film growth and desorption of the side products. All are influenced by temperature, pressure, gas mixing ratio and gas flow velocity as well as the substrate geometry and related transport mechanisms. First experimental and theoretical results will be presented.