MM 4: Structural Materials

Time: Monday 10:15–13:00 Location: H46

MM 4.1 Mon 10:15 H46

Nanoscale analysis of Ti-modified Mo-Si-B alloy to elucidate solid solution and particle strengthening — •Reshma Sonkusare[1], Torben Boll[1], Julia Becker[2], Martin Heilmaier[1], and Manja Krüger[2] — [1]Institute of Applied Materials and Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Germany — [2]Institut für Werkstoff- und Fügetechnik, Otto-von-Guericke-Universität Magdeburg, Germany

Mo-Si-B alloys are attractive high-temperature structural materials due to their high melting point (>2000C), high-temperature strength and good oxidation resistance. We found that small additions of Ti to multi-phase Mo-Si-B lead to strengthening of alloy at intermediate and high temperatures. To understand the effect of Ti on microstructure and thus mechanical properties, we investigated powder metallurgically processed Mo-7.2Si-9.7B-1.7Ti. The microstructure consists of Mo solid solution phase, intermetallic silicide phases, nanoscale oxide and silicide particles. To analyze the composition of these nanoscopic particles, atom probe tomography is required. APT reveals Ti to cause an unexpected compositional change of Mo(SS) phase. This change and an analysis of the composition and distribution of other phases combined with an investigation of the particles and elemental segregations at the grain boundaries and inside the grains improve the understanding of the solid solution and particle strengthening in the alloy and hence the mechanical behavior.

MM 4.2 Mon 10:30 H46

Intrinsic room temperature ductilisation of lean rare-earth free ternary Mg alloys — •Wassilios Delis[1], Pia Huckfeldt[1], Bengt Hallstedt[2], Pei-Ling Sun[1], Dierk Raabe[3], Sandra Korte-Kerzel[1], and Stefanie Sandlöbes-Haut[1] — [1]Institute for Physical Metallurgy and Materials Physics, RWTH Aachen, 52074 Aachen, Germany — [2]Institute for Materials Applications in Mechanical Engineering, RWTH Aachen, 52062 Aachen, Germany — [3]Max-Planck Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Mg is a lightweight structural material with a good specific strength. Unfortunately, it lacks good room temperature formability and therefore a wider commercial use of Mg is hindered. The preferred basal slip and strong basal-type texture were found to be the main reasons for the poor room temperature formability. For basal slip the von Mises' criterion is not fulfilled. Recent experimental and simulative studies tried to activate more slip systems without changing the mechanical properties with alloying approaches. Alloys containing Y and rare-earth elements showed a highly increased room-temperature ductility. Since Y and rare-earth elements are costly further research has been carried out to identify similar acting alloy systems. For this purpose, the parameter I1 SFE has been used and the system Mg-Al-Ca was identified to have a similar I1 SFE. In experiments the system indeed showed the expected increased room temperature ductility. Further research of the effects of the chemical composition on the ductilisation has now been performed.

MM 4.3 Mon 10:45 H46

PT phase transitions and spectral structure of the interacting Hatano-Nelson model — •Songbo Zhang — Stetthachrrain 20, Zurich, Switzerland

In this talk, I will discuss the Hatano-Nelson model, i.e., a one-dimensional non-Hermitian chain of spinless fermions with nearest-neighbour nonreciprocal hopping, in the presence of repulsive nearest-neighbour interactions. At half-filling, I will show two PT transitions, as the interaction strength increases. The first transition is marked by an exceptional point between the first and the second excited state in a finite-size system and is a first-order symmetry-breaking transition into a charge density wave regime. Persistent currents characteristic of the Hatano-Nelson model abruptly vanish at the transition. The second transition happens at a critical interaction strength that scales with the system size and can thus only be observed in finite-size systems. It is characterized by a collapse of all energy eigenvalues onto the real axis. I will also show that in a strong interaction regime, but away from half-filling, the many-body spectrum shows point gaps with nontrivial winding numbers, akin to the topological properties of the single-particle spectrum of the Hatano-Nelson chain.

MM 4.4 Mon 11:00 H46

Novel CDB Data Processing and Evaluation Software — •Leon Chryssos, Vassily Vadimovitch Burwitz, Lucian Mathes, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

The Coincidence Doppler-Broadening (CDB) spectrometer at NEPOMUC has recently been upgraded with six additional HPGe Detectors, bringing the total number of detectors to ten. To take full advantage of the even more capable instrument a novel data evaluation software package (STACS) is currently under development. The software can already handle and visualize the data generated by Coincidence Doppler-Broadening Spectroscopy (CDBS) and provides a wide range of tools to analyze such data. Some of the main functions include the extraction of the electron-positron annihilation photo peak from CDB spectra as well as a simple background subtraction algorithm that is able to increase the peak-to-noise ratio of the extracted photo peak further. This combined with a new multi detector CDB function, which enables the combination of the data from all 10 detectors, provides detailed information about the chemical environment of the positron annihilation site. The software capabilities were tested on W samples, to demonstrate the sensitivity for high Doppler shifts. Measurements on the precipitation hardening properties of Al alloy samples were subsequently performed and will be shown.

MM 4.5 Mon 11:15 H46

Plasticity of the Ca(Al,Mg)2 phase with variable temperature and composition — •Martina Freund[1], Doreen Andre[1], Pei-Ling Sun[1], Nicolas J. Peter[2], and Sandra Kort-Kerzel[1] — [1]Institut für Metallkunde und Materialphysik, RWTH Aachen University — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Magnesium is a promising lightweight material, but its application as cast alloys at elevated temperature is limited because of its low creep resistance. By alloying with Al and Ca different Laves phases form, which improve creep strength. While investigating largely unknown properties with respect to composition and temperature changes, a challenge is to physically relate and represent such results. Here, we explore - in addition to the specific findings - how this may be done in terms of defect phase diagrams. Due to their complex packing, Laves phases are brittle at low temperatures. In order to overcome this restriction and to study their mechanical properties and mechanisms of plasticity, we used nanomechanical testing. For the cubic CaAl2 phase, nanoindentation tests revealed a constant hardness of 5.9 +- 1.2 GPa and indentation modulus of 120.3 +- 17.9 GPa. Slip traces and cracks in the vicinity of indents were correlated with the crystal orientation and mostly corresponded to the {111} and {112} planes. Microcompression revealed deformation on {111} and {112} planes in <1-10> direction and the CRSS has been calculated as 0.97 +- 0.03 GPa and 0.96 +- 0.03 GPa, respectively. These planes and Burgers vectors were also confirmed by TEM using the g*b criterion.

15 min. break

MM 4.6 Mon 11:45 H46

Ab initio study of magneto-chemo-structural coupling at FeMn grain boundaries — •Omkar Hegde, Jörg Neugebauer, and Tilmann Hickel — Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40227 Düsseldorf, Germany

Mn segregation at Fe grain boundaries is known to be a precursor for a variety of phenomena such as embrittlement, spinodal decomposition, phase transformation, etc [1,2]. Therefore, various heat treatments are performed in experiments to control Mn decoration at grain boundaries for *segregation engineering* [1], which could alter the local magnetic state. In this direction, a thorough understanding of the connection between the local magnetic state and segregation remains elusive. In the present work, we tackle this issue by studying segregation in both the ferromagnetic state (low-temperature) and paramagnetic state (high-temperature) using ab initio-based approaches [3]. We demonstrate that the Mn segregation profile is mainly modulated by local magnetic interactions, providing new opportunities for grain boundary segregation engineering. Finally, we show that the formation of grain boundary and Mn segregation can, in turn, tune the local

magnetic transition temperature, thereby revealing a complex coupling of structure, chemistry, and magnetism.

[1] D Raabe et al., Current Opinion in Solid State and Materials Science, 18, 253-261 (2014).

[2] AK Da Silva et al., Nature communications, 9, 1-11 (2018).

[3] O Hegde et al., Physical Review B, 102, 144101 (2020).

MM 4.7 Mon 12:00 H46

Sulphation kinetics of chloride particles, corrosion potential and effect of reactive additives — •Sebastian Pentz and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

Chlorine induced high temperature corrosion leads to massive problems especially in waste-to-energy-plants, but also in biomass combustion. During the combustion process chloride containing particles are released and deposited on heat exchanger surfaces. There chlorides get converted into sulphates with a release of chlorine species which then lead to severe corrosion. In laboratory experiments we study the conversion kinetics under various conditions like temperature, particle size or gas composition. Both the sulphation reaction and the rate of subsequent corrosion show an Arrhenius dependency on temperature, a linear dependence on time, on particle surface and on partial pressure of SO2. The addition of reactive additives can strongly influence this reaction and consequently the release of chlorine species: Adding iron oxide (e.g. Fe_2O_3) results in a strong acceleration of the sulphation process due to catalysis of the reaction from SO_2 to SO_3. On the other hand, a reduction of the sulphur content in the reaction atmosphere by desulphurising species like calcium oxide slows down the sulphation reaction and reduces the amount of released chlorine compounds.In lab experiments, chlorides (mixed with additives) are applied to 16Mo3 steel samples and exposed to a flowing reaction atmosphere in a tube furnace.Support by Federal Ministry for Economic Affairs and Climate Action on the basis of a decision by the German Bundestag.

MM 4.8 Mon 12:15 H46

Influence of oxygen and carbon on the chemistry at the niobium/alumina interface in a refractory composite material — •Michael Eusterholz[1], Torben Boll[1], Alexander Kauffmann[1], Reshma Sonkusare[1], Vincent Ott[1], Julian Gebauer[1], Bastian Kraft[1], Anja Weidner[2], Michael Stüber[1], Sven Ulrich[1], and Martin Heilmaier[1] — [1]Karlsruhe Institute of Technology (KIT) — [2]TU Bergakademie Freiberg (TUBAF)

High-temperature processes such as steel casting impose harsh conditions on materials, which thus require excellent properties, including creep strength and resistance to thermal shock. Composites based on coarse-grained refractory metals and refractory ceramics promise superior performances due to adjustable mechanical and electrical properties.

Conventionally sintered composites from technical grade raw materials of α-Al_2O_3 and Nb include impurity elements that form carbides alongside oxides during synthesis. To understand the principles of formation, we investigate α-Al_2O_3 substrates sputter-coated with Nb as model materials beside the technical grade material. As the latter is subjected to carbon and oxygen containing gases during sintering, we compare the effect of oxygen and carbon overexposure on the ceramic-metal interface and contrast these results with a heat treatment with unaffected interface. Electron microscopy techniques elucidate the microstructure, while atom probe tomography advances the understanding of nano-scale phase formation at the phase boundary which are decisive for the material properties and corrosion resistance.

MM 4.9 Mon 12:30 H46

Oxidation mechanisms of SMART alloys and MAX phases — •Anicha Reuban[1,2], Jesus Gonzalez-Julian[1,2], Ivan Povstugar[1], Andrey Litnovsky[1,3], and Christian Linsmeier[1] — [1]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Mineral Engineering, RWTH Aachen University, 52064 Aachen, Germany — [3]Moscow

Concentrated Solar Power (CSP) is a sustainable energy technology where sunlight is focused on a solar receiver and the thermal energy is used to generate electricity. The receiver must withstand temperatures greater than 1000 °C, be resistant to oxidation by air and/or corrosion by molten salts and and maintain its properties over time. Self-passivating SMART alloys, originally designed for the fusion reactor, are resistant to plasma sputtering and can suppress oxidation in case of an accident with air ingress, up to 1000 °C. MAX phases, a bridge between metals and ceramics, are lightweight, easily machinable materials, oxidation- and corrosion-resistant up to 1400 °C. To understand the oxidation mechanisms in these materials, it is important to obtain nanoscale information using advanced characterization techniques such as Atom Probe Tomography (APT). According to the APT analysis of the SMART alloy W-Cr-Y, Y segregates at oxide grain boundaries while in the alloy it forms Y-O precipitates. Further analyses are being performed to get more information about the role of Y in the oxidation process. Electron microscopy is used along with APT for a correlative approach to nanoscale characterization.

MM 4.10 Mon 12:45 H46

Development of Tungsten fiber reinforced tungsten (Wf/W) using yarn based textile preforms — •Alexander Lau[1], Jan Willem Coenen[1], Daniel Schwalenberg[1], Yiran Mao[1], Alexis Terra[1], Leonard Raumann[1,2], Michael Treitz[1,4], Johann Riesch[3], Hanns Gietl[3,4], Beatrix Göhts[1], Christian Linsmeier[1], Katharina Theis-Bröhl[2], Till Höschen[3], and Phillip Huber[5] — [1]Forschungszentrum Jülich GmbH, Institut für Plasmaphysik, 52425 Jülich — [2]Hochschule Bremerhaven, 27568 Bremerhaven — [3]Max-Planck-Institute for Plasma Physics, 85748 Garching b. München — [4]Technische Universität München, 85748 Garching — [5]RWTH Aachen University, 52062 Aachen, Germany

The focus of this work is the development of a new composite material, that has to withstand the immense heat and particle fluxes in future fusion reactors. The wall material is based on the element tungsten, which already shows a very high compliance with the requirement profile in its pure form. Pure tungsten is inherently brittle below the DBTT and cracks could lead to a complete failure of the wall material. To counter this problem, extrinsic strengthening mechanisms were tested with new fabric types, based on radially braided yarns with seven core- and 16 sleeve filaments. These yarns were coated with an Yttriumoxide interface by Magnetron-sputtering and then further processed with chemically vapor deposited tungsten in a six-layer structure to form a solid composite material. This sample was analysed optically and got mechanically tested in a three-point bending test.