MM 37: Topical Session: Defect Phases II

Time: Thursday 10:15–13:00 Location: SCH A 216

Topical Talk MM 37.1 Thu 10:15 SCH A 216

Structural and chemical atomic complexity of lattice defects – From defect phase diagrams to properties of intermetallics — Martina Freund, Xie Zhuocheng, Lukas Berners, Pei Ling Sun, Stefanie Sandlöbes-Haut, and •Sandra Korte-Kerzel — Institut für Metallkunde und Materialphysik, RWTH Aachen University

Two approaches in materials physics have proven immensely successful in alloy design: First, thermodynamic and kinetic descriptions for tailoring and processing alloys to achieve a desired microstructure. Second, crystal defect manipulation to control strength, formability and corrosion resistance. However, to date, the two concepts remain essentially decoupled. A bridge is needed between these powerful approaches to achieve a single conceptual framework. Considering defects and their thermodynamic state holistically as defect phases, provides a future materials design strategy by jointly treating the thermodynamic stability of both, the local crystalline structure and the distribution of elements at defects.

Here, we will report our work on intermetallics, which are complex already in their underlying crystal structure, to reveal active deformation mechanisms and their dependence on both structure and chemical composition.

MM 37.2 Thu 10:45 SCH A 216

The synthesis and studies of unique oxygen structure on silica-aluminate catalysts — •Linfeng Su[1], Xu Chen[2], Huaping Zhao[1], Zhiyi Lu[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key Laboratory of Advanced Fuel Cells and Electrolyzers Technology of Zhejiang Province, Ningbo Institute of Materials Technology and Engineering, CAS, Zhejiang, 315201, PR China

To promote the application of silica-aluminate catalysts in catalytic reactions, the unique active oxygen structures on the surface of silica-aluminate were investigated. 4A molecular sieves were prepared with oxygen-rich vacancies of various contents and different chemical environments. Three different types of oxygen vacancies (due to the covalent and coordination bonds of O) on the surface have different mechanisms in catalytic reactions, and the specific structures exhibit the best catalytic activity (87.5% removal rate of pollutants within 6 min in catalytic ozonation). Moreover, silica-aluminate mullite containing abundant neo-oxygen structure (unique bridging oxygen) was successfully prepared at a low preparation temperature. The abundant oxygen structure in silica-aluminate leads to abundant unique bridging oxygen structures with high catalytic activities (81.2% removal rate of pollutants within 15 min under low ozone concentration). The research on the unique oxygen structure of silicate-aluminate provides theoretical guidance for the design and synthesis of catalysts with high catalytic activities for future industrial applications.

MM 37.3 Thu 11:00 SCH A 216

Understanding corrosion phenomena based on surface phase diagrams for Mg alloys in contact with water — •Jing Yang, Mira Todorova, and Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Max-Planck-Strasse 1, D-40237 Düsseldorf, Germany

Defect phases formed at alloy surfaces and interfaces govern their chemical and mechanical behavior. Constructing phase diagrams from ab initio modeling provides valuable information for understanding the microscopic mechanisms of surface and interface processes. In this work, we apply this approach to study the aqueous corrosion of magnesium alloyed with Al and Ca, an important structural material for the automotive and aerospace industries. Constructing defect phase diagrams for the passive film formed on the magnesium surface, we analyze how the Al and Ca alloying atoms evolve during the corrosion process and how they impact the corrosion resistance of the magnesium alloy. In particular, we resolve the cause of Al enrichment in the passive film, which has been recently observed in experiment. Based on these examples we discuss how defect phase diagrams can help us to better understand microscopic chemical processes under realistic conditions.

MM 37.4 Thu 11:15 SCH A 216

Ab-initio informed CALPHAD modelling of grain boundaries — •Tobias Spitaler[1], Rishi Bodlos[2], Daniel Scheiber[2], and Lorenz Romaner[1] — [1]Montanuniversität Leoben, Department Werkstoffwissenschaft, Leoben, Österreich — [2]Materials Center Leoben Forschung GmbH, Leoben, Österreich

The CALPHAD method is an important tool in material science to calculate phase diagrams and to predict phase stabilities of complex systems. Based on a model of the Gibbs Free energy of the bulk phases as function of composition, pressure and temperature the thermodynamic equilibrium quantities can be calculated with computer programs. In materials grain boundaries play an important role for mechanical properties and grain growth. Alloying elements often tend to segregate from or to the grain boundary, changing the properties of the grain boundary for example by weakening or strengthening the cohesion or by preventing grain boundary movement, which can lead to stabilisation of a nano-crystalline structure.

We therefore devise a formulation of the grain boundary Gibbs Free energy within the compound energy formalism with the goal to obtain the grain boundary state parameters such as composition and grain boundary area. We use DFT calculations to explore energy configurations of grain boundaries and couple them to thermodynamic models to investigate solute segregation and its impact on the grain boundary energy. With these results we can provide grain boundary phase diagrams and address thermodynamic nanocrystalline stability in metallic alloys.

15 min. break

Topical Talk MM 37.5 Thu 11:45 SCH A 216

Density-based Grain Boundary Phase Diagrams — •Reza Darvishi Kamachali — Federal Institute for Materials Research and Testing (BAM)

Phase diagrams are the roadmaps of material design yet primarily developed and discussed for defect-free bulk phases. Real microstructures, however, also contain large populations of defects, such as grain boundaries, which show their own distinct phase behavior. Recently, CALPHAD-integrated density-based phase diagrams were proposed for studying segregation and phase evolution in grain boundaries. In this method, the connection to available bulk thermodynamic data allows rapid assessment of grain boundary phase behavior. In this talk, density-based phase diagrams of several binary and ternary alloy systems will be discussed, with direct implications for alloy and microstructure design. The significance and integration of elastic energies to the density-based model will be presented. It will be shown that Cu segregation and segregation transition in Al-Cu and Al-Cu-Mg systems can be explained by the presence of solutes' elastic interactions with grain boundaries.

MM 37.6 Thu 12:15 SCH A 216

Learning chemistry dependence of grain boundary segregation energies — •Christoph Dösinger[1], Daniel Scheiber[2], Oleg Peil[2], Vsevolod Razumovskiy[2], and Lorenz Romaner[1] — [1]Montanuniversität Leoben, Department of Materials Science, Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria

The grain-boundary segregation energy (E_{seg}) is the central quantity for describing the process of grain-boundary segregation which influences fracture. Usually, to obtain highly accurate values for E_{seg}, density functional theory is employed, which incurs high computational costs. This makes it impractical to do a thorough study of segregation to multiple grain-boundaries for a range of solutes. To reduce the number of calculations needed for such a complete description, we apply machine learning methods to density functional theory data. By using separate sets of descriptors for the local atomic environment and the solute types, we fit a model based on gaussian process regression. This approach is evaluated on a comprehensive data-set for E_{seg} in tungsten. The tests indicate that the model has the ability to extrapolate to solutes which are not contained in the training data.

MM 37.7 Thu 12:30 SCH A 216

Rationalising the impact of experimental preparation routes

on impurity content in Pd nano-aerogels using ab-initio phase diagrams — •Mira Todorova, Su-Hyun Yoo, Poulami Chakraborty, Tilmann Hickel, Se-Ho Kim, Baptiste Gault, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

Recent advances of experimental techniques with atomic resolution enable us to analyze the structure and composition of samples at the sub-nanometer scale, providing information about contamination with impurities and their distribution. Understanding the factors which govern the ingress, amount and distribution of contaminating elements, opens routes to both improving the sample quality and their utilization in targeted design to achieve a desired functionality. Using an ab-initio based thermodynamic approach and surface phase diagrams we unravel the impact of preparation conditions on experimental observations and materials properties. The power and the performance of these ab-initio based thermodynamic concepts will be highlighted using the example of impurity incorporation during wet-synthesis of nano-aerogels, specifically Na and K incorporation into grain boundaries [JACS 144, 987 (2022)] and B into the bulk [Adv. Mater. 2203030 (2022)] of Pd nano-aerogels.

MM 37.8 Thu 12:45 SCH A 216

Influence of stoichiometric change on plasticity in the Ca(Al;Mg)2 C15-Laves Phase — •Martina Freund[1], Peiling Sun[1], Carsten Thomas[2], Deborah Neuss[3], Michael Feuerbacher[2], Marcus Hans[3], and Sandra Korte-Kerzel[1] — [1]Institut für Metallkunde und Materialphysik, RWTH Aachen University — [2]Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen und Peter-Grünberg Institut Forschungszentrum Jülich GmbH — [3]Materials Chemistry, RWTH Aachen University

Magnesium is a promising material for light weight applications but is strongly limited because of its low room temperature ductility and low creep resistance. By alloying with Al and Ca dif-ferent Laves phases form, which improve creep strength properties. We did investigations of the stoichiometric C15 Laves phase, finding slip on {111} and {112} planes with the same ac-tivation frequency and approximately same CRSS values. The influence of the stoichiometry regarding the plasticity was analysed using a sample with 6at.-% Mg, by nanoindentation tests, APT and TEM. Hardness and indentation modulus values were in the same range for all indented orientations. Comparing this to the stoichiometric one, the hardness has shown a slight increase around 1 GPa. Changes of plasticity were seen by analysing resulting slip lines. Most activated slip planes were the {112} planes, followed by the {110}. APT was done for both, the stoichiometric and the off-stoichiometric, to evaluate the local chemistry on {112} slip planes. Ultimately, we aim to reveal the connection between the local chemical potential and motion of dislocations on different slip planes.