MM 13: Topical Session Designing Innovative Structural Materials and Steels IV

Time: Monday 16:00–17:45 Location: H4

MM 13.1 Mon 16:00 H4

Atomic-scale quantification of the mechanisms underlying solid solution hardening — •Johann von Pezold, Martin Friák, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck Strasse 1, 40237 Düsseldorf

The increase in the initial flow stress of metals by the introduction of impurity atoms (solid solution hardening) is generally accounted for by a combination of the size (parelastic) and elastic (dielastic) mismatch between the host and the solute atoms. In this study we have investigated the mobility of edge dislocations in aluminum in the presence of impurity atoms using Molecular Dynamics (MD) simulations in order to quantify the relative contributions of the two effects. The Al host was described by an embedded-atom-type potential (EAM), while the impurity atoms were introduced by overlaying the EAM potential with a Lennard-Jones potential on the impurity sites, which allowed us to independently vary the size- and elastic mismatch between the metal host and the defect atoms. Our results suggest that the size mismatch is the predominant contribution to solid solution hardening, while the dielastic interaction is only of secondary importance. Based on this insight we discuss a multiscale approach for the determination of optimum hardening conditions from ab initio calculations.

MM 13.2 Mon 16:15 H4

Stability and mobility of hydrogen in the vicinity of point and extended defects in bcc-Fe — •Jutta Rogal, Yaojun A. Du, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

The detrimental effect of hydrogen on materials properties poses problems for many applications. Hydrogen embrittlement of iron and steels has been studied extensively in experiments and theory, but due to the complexity of the problem it is still not fully understood. Two of the most discussed mechanisms for hydrogen embrittlement are the HEDE and HELP mechanisms. To address these mechanisms from a microscopic point of view it is important to obtain a detailed understanding of the stability and mobility of hydrogen in the vicinity of point and extended defects.

We have performed density-functional theory calculations to investigate the solubility and diffusion behaviour of hydrogen close to grain boundaries and vacancies in bcc-Fe. In bcc-Fe, hydrogen at a grain boundary is energetically favoured compared to the bulk region. Together with the very low diffusion barriers of hydrogen in bcc-Fe this may lead to a local accumulation of hydrogen around the defect even for rather small H concentrations. Employing kinetic simulations we investigate the diffusion of hydrogen in the presence of a defect and analyse the time evolution of the local hydrogen distribution.

MM 13.3 Mon 16:30 H4

In-situ investigation of precipitation in AA7449 friction stir welds using high energy SAXS — •Torben Fischer, Peter Staron, Luciano Bergmann, Jorge F. dos Santos, and Andreas Schreyer — GKSS Research Centre, 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 friction stir welded, thermo-mechanical processes alter the base metal microstructure and properties. The result is 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 welding can only be registered by in-situ experiments. Therefore, a new transportable FSW system 'FlexiStir', for in-situ measurements was developed by GKSS. The in-situ experiments with the FlexiStir took place at the GKSS high-energy synchrotron beamline HARWI II at HASYLAB. Small-angle X-ray scattering (SAXS) at high photon energies was used to obtain spatial resolved results on volume fractions and sizes of precipitates at different locations in the weld zone.

MM 13.4 Mon 16:45 H4

Phase-contrast imaging with an x-ray grating interferometer in materials science using noncoherent synchrotron radiation — •Julia Herzen[1], Felix Beckmann[1], Tilman Donath[2], Malte Ogurreck[1], Stefan Riekehr[1], Christian David[2], Franz Pfeiffer[3], Astrid Haibel[1], and Andreas Schreyer[1] — [1]GKSS Research Centre, Geesthacht, Germany — [2]Paul Scherrer Institute, Villigen PSI, Switzerland — [3]Technische Universität München, Munich, Germany

Phase-contrast imaging with a hard x-ray grating interferometer is used to increase contrast for weak absorbing materials. It is a well established imaging method to visualize soft tissue in many medical and biological applications. Here we present the approach of using this method in the field of materials science, especially in imaging of new light-weight materials like magnesium and aluminium alloys. We show that more information from a single x-ray projection image can be gained by combining the different contrasts obtained by this imaging method simultaneously. This information can be used to optimize advanced joining techniques for such materials.

MM 13.5 Mon 17:00 H4

Metastable phase formation in undercooled Fe-Cr-Ni alloy melts — Thomas Volkmann[1], Wolfgang Löser[2], and •Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), D-51170 Köln — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), D-01171 Dresden

The solidification behaviour of undercooled Fe69Cr31-xNix melts, which represents the basis for the technically important stainless steels, was investigated in a wide composition range (7 at.% < x < 22 at.%) with respect to the competitive formation of ferrite (bcc) and austenite (fcc). The electromagnetic levitation technique was used for undercooling of bulk samples. The primary solidifying phase was identified by the analysis of time-resolved recalescence profiles that were detected by a fast responding photo diode at a rate of 1 MHz. Under equilibrium conditions the solidification mode changes from ferrite to austenite if the atomic fraction ratio of Ni/Cr = 0.5 is exceeded. It is shown that crystallization of bcc phase is preferred even at compositions where bcc is metastable. With rising undercooling a transition from primary fcc to primary bcc solidification occurs at a critical undercooling. The experimental results are compared to the predictions of the classical nucleation theory and an improved theory taking into account a finite thickness of the interface between the nucleus and the undercooled melt.

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MM 13.6 Mon 17:15 H4

***Ab initio* molecular dynamics study of interface layer formation at aluminum oxide/silicon nitride interfaces** — •Steve Schmerler and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

Ab initio molecular dynamics techniques are a powerful tool for the study of dynamic effects in materials such as vibrational properties as well as structural phase transitions and phase formations.

We present results from molecular dynamics studies of aluminum oxide/silicon nitride interfaces at elevated temperatures. The formation of new interface layers and diffusion properties are discussed.

We would like to thank the DFG for financial support within the DFG Priority Program 1236: *Strukturen und Eigenschaften von Kristallen bei extrem hohen Drücken und Temperaturen*

MM 13.7 Mon 17:30 H4

Ab-initio study of structural stability of Fe-B phases — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

Boron is added to steels in small concentrations to improve strength, creep resistance and corrosion properties. However, the impact of boron can be beneficial or detrimental, depending on the steel composition, the boron concentration and the fabrication process itself. A conclusive picture of borons' influence on the mechanical properties and operational characteristics of steel is still missing. A first step

towards an atomistic understanding of boron in steels is the study of structural stability of Fe-B bulk phases.
To this end, we performed spin-polarized density-functional theory (DFT) calculations of the Fe-B system. In particular, we calculated the heat-of-formation of Fe-B for a large set of structures. The set of investigated crystal structures is based on a collection of experimentally observed phases of transition metals with light elements. We compare our DFT results to the experimental phase diagram of Fe-B and discuss the interaction of boron in iron.