MM 40: Topical Session: Interface-dominated phenomena - Solutes at Interfaces I

Time: Wednesday 15:45–17:00 Location: IFW A

Topical Talk MM 40.1 Wed 15:45 IFW A

Using interfaces to move solute atoms and using moved atoms to stop interfaces in steels — •Sybrand van der Zwaag — TU Delft, Delft, the Netherlands

Diffusional phase transformations in steels can involve the partitioning of substitutional alloying elements at the moving austenite-ferrite interface. Under normal isochronal or isothermal annealing conditions the local solute enrichment is spatially coupled to (one side of) the interface at all times. However, in the cyclic partial phase transformation approach, the direction of the moving interface is reverted periodically and the enriched region and the crystallographic interface separate due to a difference in mobility. Hence, reversing the direction of the interface allows for the creation of narrow (nm wide) regions with a higher concentration of substitutional alloying elements within the crystallographically unaffected parent austenitic matrix. Multiple passes towards the enriched rim left behind in the first partial transformation cycle will increase the local enrichment even further. The enriched rim manifests itself as a (chemical) barrier and can block the interface upon final cooling for as much as 150 K. The interface motion and blocking effects are analysed using dilatometry, laser scanning confocal microscopy and Transmission Electron Microscopy.

The chemical boundary engineering (CBE) concept has then been used to create steels in which the sharp boundaries of enriched domains locally halt the advancing martensitic phase fronts, resulting in a nanostructured multiphase steel with exceptional mechanical properties.

MM 40.2 Wed 16:15 IFW A

Atomic scale structure and segregation behavior at Σ5 tilt grain boundaries in bcc iron — •Ali Ahmadian, Xuyang Zhou, Christian H. Liebscher, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) are two-dimensional defects, which determine the mechanical as well as physical properties of polycrystalline materials. Segregation of impurities, such as phosphorous, to GBs can reduce their cohesive strength and with this lead to embrittlement of a material. By introducing other impurities such as carbon, the segregation tendency of phosphorous can be suppressed. It is under debate whether boron has the same effect as carbon and how a co-segregation of both elements influences GB properties [1]. In this work, we investigated ferritic Fe-2wt%Al bicrystals grown by a modified Bridgeman technique. The global structure of the GB is characterized by electron backscatter diffraction, revealing a symmetric Σ5 [001] (310) tilt GB. Aberration-corrected scanning transmission electron microscopy experiments showed kite-type structural units as predicted by atomistic simulations by Scheiber et al. [2]. However, the atomic structure of the GB also contains other defects such as facets or steps, leading to different local reconstructions. In combination with atom probe tomography experiments, a clear segregation of both carbon and boron is observed, while aluminium is depleted at the boundary. The latter one is in contradiction to DFT calculations, where a clear segregation of aluminium was predicted. [1] C. M. Liu et al., Metall Trans A 23 (1992) [2] D. Scheiber et al., MODEL SIMUL MATER SC 24 (2016)

MM 40.3 Wed 16:30 IFW A

Correlative study of grain boundary segregation in nanocrystalline copper-nickel alloys — •Felix Fischer, Rüya Duran, and Guido Schmitz — Institute for Materials Science, University of Stuttgart, Germany

Nanocrystalline material properties are dominated by grain boundaries (GB). In nanocrystalline copper-nickel alloys, which have high corrosion resistance, thermal conductivity and fabricability, segregation of copper to GBs is energetically preferred and was previously quantified in simulations. In these simulations the values for excess segregation depend highly on grain boundary structure, therefor transmission electron backscatter diffraction (t-EBSD) and atom probe tomography (APT) measurements are carried out on prepared nanocrystalline tips.

t-EBSD allows an evaluation of the grain orientations and thus the GB types, while APT gives an atomically-resolved digital reconstruction of the measured tip. Combing these two methods, the segregation of copper to GBs can be correlated to the GB type, alloy concentration as well as the annealing temperature and furthermore compared to simulated segregations. By applying molecular dynamic simulations, additionally, the excess segregations of so far unevaluated GBs can be obtained and directly compared to experimental results.

The presentation will elucidate in detail the experimental procedure and shortly mention the used simulation methods from which the correlations of GB segregation to GB type, concentration and temperature are determined and also compared between theory and experiment.

MM 40.4 Wed 16:45 IFW A

The effect of grain boundary segregation on embrittlement: recent trends and open questions — Pavel Lejček[1] and •Mojmir Šob[2,3,4] — [1]Inst. Phys., Acad. Sci. Czech Rep., Prague — [2]Masaryk Univ., Fac. Sci., Dept. of Chem., Brno, Czech Rep. — [3]Inst. Phys. Mat., Acad. Sci. Czech Rep., Brno — [4]Central Europ. Inst. Technol., CEITEC MU, Masaryk Univ., Brno

To elucidate the effect of individual solutes on embrittlement of various base materials such as steels and nickel-base superalloys, grain boundary and surface segregation was extensively studied in many laboratories. Unfortunately, the values of the segregation energy of a solute at grain boundaries as well as at the surfaces obtained by various authors sometimes differ by more than one order of magnitude: such a difference is unacceptable as it cannot provide us with representative view on the problem of material temper embrittlement Here we summarize the available data on interfacial segregation and embrittlement of various solutes in nickel and bcc iron and critically discuss their reliability, assessing also limitations of individual approaches employed to determine the values of segregation and strengthening/embrittling energies. We demonstrate that theoretical approaches are limited by the size of the computational repeat cell used for the calculations of the segregation energy. On the other hand, the change in the grain boundary cohesion (strengthening/embrittling energy) may be obtained with a reasonable accuracy. For many impurities, there is lack of experimental segregation data. Therefore, many calculated results are theoretical predictions which may motivate future experimental work.