MM 6: Topical Session Interface-Dominated Phenomena - Thermodynamics

Time: Wednesday 10:00–11:00 Location: H8

Invited Talk MM 6.1 Wed 10:00 H8

CALPHAD-informed density-based grain boundary thermodynamics — •Reza Darvishi Kamachali[1], Lei Wang[1], Linlin Li[2], Anna Manzoni[1], Birgit Skrotzki[1], and Gregory Thompson[3] — [1]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin — [2]State Key Laboratory of Rolling and Automation, Northeastern University, Shenyang 110819, PR China — [3]University of Alabama, Department of Metallurgical Materials Engineering, 35487 Tuscaloosa, AL, USA

The Gibbs free energy of a grain boundary is a complex thermodynamic function of temperature, pressure, and composition. These complexities add to the intrinsic crystallographic and chemical constraints imposed by the adjacent bulk phase. Recently we have proposed a density-based model for assessing grain boundary thermodynamics that enables a CALPHAD-informed description of the grain boundary. As such, the Gibbs free energy of the grain boundary is directly linked to available CALPHAD thermodynamic data. In this talk, new aspects of interfacial segregation and phase transformation are revealed by benchmarking the current model for various experimental cases, including several steels, high-entropy alloys and aluminum alloys. The effects of elastic interactions on the grain boundary segregation and the application of the model to a nanocrystalline Pt-Au alloy, with numerous grain boundaries of various characters, will be discussed.

MM 6.2 Wed 10:30 H8

Methods for Gibbs triple junction excess determination: Ti segregation in CoSi2 thin film — •Hannes Zschiesche, Ahmed Charai, Claude Alfonso, and Dominique Mangelinck — CNRS, IM2NP, Faculté de Saint-Jérôme, Aix-Marseille Université, Marseille, France

Triple junctions (TJs) are present in poly crystalline material where three grain boundaries join together. They influence directly the thermodynamics and kinetics of the material and thereby its properties. Thus, their description by geometric and thermodynamic parameters is of great interest. One of these parameters is the Gibbs TJ segregation excess. Eich et al., Acta Mater, 2018 predicted TJ excess in a Fe-Cr alloy based on simulations. However, to compare such predictions on experimentally acquired TJs methods are needed for the determination of Gibbs TJ segregation excess.

We propose methods to determine Gibbs TJ segregation excess in an atomically resolved 3D volume where single atom counting is possible, as provided by atom probe tomography (APT). Firstly, we test the methods on a simulated model volume in which the excess value is known. Further, we investigate an APT volume of CoSi2 thin film that contains three grain boundaries and a TJ which show segregation of Ti. CoSi2 is well known as contact material in microelectronics and can grow in epitaxy on Si by the introduction of a Ti interlayer. The developed methods allow to quantify the Ti excess at the CoSi2 TJ.

This work offers new possibilities for fundamental characterization of materials and an example of its application.

MM 6.3 Wed 10:45 H8

A quantum-mechanical study of impact of vibrational entropy on the segregation of Cu to antiphase boundaries in Fe_3Al — •Martin Friák[1,2], Miroslav Černý[2,3], and Mojmír Šob[4,1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, Czech Republic — [3]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have performed an *ab initio* study of segregation of Cu atoms towards antiphase boundaries (APBs) in Fe_3Al. The Cu atoms are predicted to segregate towards the studied APBs (the APB energy is then equal to 84 mJ/m^2) but the related energy gain is only 4 meV per Cu atom. Both Cu atoms (as point defects) and APBs (as extended defects) have their specific impact on local magnetic moments of Fe atoms (and they non-linearly combine when both types of defects are present). We have also performed phonon calculations and found all studied states mechanically stable. The band gap in phonon frequencies of Fe_3Al is barely affected by Cu substituents but reduced by APBs. The phonon contributions into segregation-related energy changes are significant, ranging from a decrease by 16 % at T = 0 K to an increase by 17 % at T = 400 K (changes with respect to the segregation-related energy difference between static lattices). Further, we have found non-linear trends in changes induced by the Cu segregation in the phonon entropy and phonon energy.