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Segregation Effects at Internal Interfaces in Alloys: Atom-Probe Tomographic Experiments and Simulations[1]

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This talk first focuses on experimental studies of solute segregation effects on an atomic scale of solute segregation at grain boundaries (GBs) and heterophase interfaces employing atom-probe field-ion microscopy and three-dimensional atom-probe tomography; both instruments provide a spatial resolution of ca. 0.2 nm in direct space. It is demonstrated that the Gibbsian interfacial excess of solute at an internal interface depends on its five macroscopic degrees of freedom (DOFs), which is consistent with J. Cahn's local phase rules for GBs and heterophase interfaces. Experimental data is presented for GBs in metallic alloys (e.g. Fe-Si, Al-Sc-Mg, Ni-Al-Cr alloys), and metal silicide/silicon and indium arsenide heterophase interfaces. Secondly, atomic-scale simulations will be presented of GB segregation in binary metallic alloys described by embedded-atom method potentials employing Metropolis algorithm Monte Carlo simulations, which further demonstrate the intimate relationships between GB structure, on an atomic scale, and the Gibbsian interfacial excess of solute. It is also shown how the microscopic DOFs of a GB affect the Gibbsian interfacial excess of solute. Additionally, the results of atom-probe tomographic studies of segregation effects at heterophase interfaces between the gamma (f.c.c.) and gamma prime ($L1_2$ structure) heterophase interfaces in Ni-Al-Cr alloys are discussed and compared in detail with the results of lattice kinetic Monte Carlo (LKMC) simulations, which involves a vacancy mediated diffusion mechanism. The LKMC simulation allow us to explain the role of vacancy-solute binding energies on the observed concentration profiles of Ni, Al, and Cr between the gamma and gamma prime phases. These detailed experimental and simulation studies of segregation effects result in a relatively new atomistic picture of segregation at internal interfaces that differs from the conventional wisdoms found in the literature concerning segregation.

[1]NSF, DOE, ONR