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Adsorption Transitions and Microstructural Evolution

W.D. Kaplan[1]
[1]*Department of Materials Science & Engineering, Technion – Israel Institute of Technology, Haifa, Israel*

Abstract: It is recognized that interfaces (including free surfaces, grain boundaries (GBs), and interfaces between dissimilar phases) can be described using diffuse interface theory, where the structure and chemistry of interfaces can go through 2-D transitions between thermodynamic states (termed complexions) in order to minimize the interface energy. As such, complexions for interfaces are analogous to phases in the bulk. To date, almost all experimental studies on potential complexion transitions have been conducted on GBs in single phase polycrystalline systems, which by definition are not at equilibrium. Similar questions have been raised regarding interfaces in thin film studies, where the deposition process may be very far from equilibrium.

This presentation will focus on an experimental approach to address the structure, chemistry, and energy of complexions at interfaces which are fully equilibrated, from which it can be demonstrated that a change in complexion minimizes interface energy. This will be compared with solid-liquid interfaces, where a region of ordered liquid exists adjacent to the interface at equilibrium, and the details of a solid-solid interface where the reconstructed interface structure accommodates lattice mismatch for a nominally incoherent interface. These three systems will be compared to known reconstructed solid surfaces, which can also be described as complexions, within a more generalized Gibbs adsorption isotherm.

From this basis, an example of the use of complexions to control grain growth dynamics in polycrystalline alumina will be presented, where experimentally measured dopant solubility limits at the sintering temperature are used to confirm if equilibrium grain boundary (GB) segregation or enrichment defines GB mobility. Analysis of GB mobility of alumina as a function of dopant concentration has shown that some segregating dopants, associated with complexion transitions, increase the GB mobility, i.e. the opposite of solute-drag.