Computation and Data Science for a Rigorous Treatment of Grain Boundary Segregation in Polycrystals

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Although grain boundary segregation is an extremely widely known phenomenon with practical impacts on virtually all polycrystalline materials, it is difficult to model rigorously. It is therefore often studied by invoking major simplifying assumptions, or addressed in a highly targeted manner where specific problems are addressed without generality. This talk will overview our recent work aimed at a rigorous and comprehensive thermodynamic treatment of grain boundary segregation in polycrystalline metals. The approach begins with studies of the wide spectrum of grain boundary sites that compete for segregant, and uses methods of data science to “learn” that spectrum for many alloys. Such learning methods dramatically simplify the vast grain boundary environment space as well as the alloy space, allowing rapid computation of grain boundary segregation “atlases” for many materials. Combining machine learning with multiscale modeling, this approach is developed in a manner that is rigorous down to the electronic level. This approach is also amenable to treatment of more complex effects including vibrational entropy and solute-solute interactions, which makes it applicable across the whole phase diagram of a given alloy system, i.e., far from the dilute limit and up to high temperatures as well.