591e Effect of Diffusion on Precipitate Nucleation and Growth

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The classical theory of nucleation and growth of a new phase is interface-limited and works well when the initial and final phases have the same composition. However, many phase transformations of practical interest have initial and final phases of different composition and long-range diffusion needs to be treated correctly. Recently, Kelton extended the classical theory via a "coupled flux" model for the nucleation and growth of a precipitate, coupling the interfacial and long-range diffusive fluxes (Kelton, Acta Mater. 49 (2000), pp. 1967). To test his model, we use Kinetic Monte Carlo simulations of a lattice gas model to study the effect of the coupled interfacial and diffusional fluxes on the nucleation and growth of a precipitate. Our simulations show several of the distinct features predicted by the coupled flux model, most importantly, a depletion of monomers near to precipitates that are larger than the (nucleation) critical size and an enrichment near to precipitates that are smaller than the critical size. Due to this enrichment and deletion, the growth rate of clusters larger than the critical size and the shrinking rate of clusters smaller than the critical size can be reduced several orders in magnitude for very low diffusion rates. The diffusion effect is larger in the growth of clusters larger than the critical size than in the shrinking of clusters smaller than the critical size.