

Simulating Encapsulated Nanoparticles; Accelerating Dynamical Simulation.

Dean C. Sayle^{1,*}, Graeme W. Watson², Steve C. Parker³

¹DEOS, Cranfield University, RMCS, Shrivenham, Swindon, UK, sayle@rmcs.cranfield.ac.uk

²Dept. of Chemistry, Trinity College, Dublin 2, Ireland.

³Dept. of Chemistry, University of Bath, Claverton Down, Bath, Avon, UK

The nature of impurities within a material is influenced by the material microstructure. However, it is not always clear whether impurities exist as very small nanocrystals, i.e. not true solid solutions, but micro mixtures. Clearly, an important issue since the nature of such impurities will reflect upon the material properties. Here, we use simulation techniques to address such issues and consider two themes:

- a/ Solid Solutions: Dispersed impurities within a particular microstructure.
- b/ Encapsulated Nanoparticles: Aggregated impurities within a particular microstructure

We describe simulation strategies, which can generate the atomistic microstructure of supported nanoparticles and thin films within a single *mesoscopic* cell including: dislocation networks, grain-boundaries, lattice slip, epitaxial configurations, surfaces morphologies, low interfacial densities and ion migration across interfacial boundaries. These models are then used as a framework, to establish the effect of the microstructure on the nature of impurities within the material. We consider both solid solution formation and encapsulated nanoparticle (aggregated impurities).

The evolutionary simulation procedure: Amorphisation and Recrystallisation, entails forcing the material to first amorphise followed by a recrystallisation step facilitating the evolution of the structural features (microstructure). Amorphising the system enables the potential energy barriers associated with ion migration to be lowered considerably compared with the crystalline material. Consequently, the ions have sufficient mobility to rearrange into low energy configurations, within the short timescales (generally of the order of nanoseconds) accessible to typical dynamical simulations. Indeed, the mobility is similar to that observed within a melt, enabling appreciable exploration of the potential energy surface, using current computational resources. Conversely, dynamical simulation, as applied to a crystalline ionic solid, would give no appreciable ionic mobility; rather the ions would simply vibrate about their lattice positions. The strategy facilitates a phenomenal acceleration of the dynamical simulation, thereby bridging the timescale gap.