Structure and stability of crystalline interfaces

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The molecular simulation group are active in simulating the nucleation, growth and assembly of molecular crystals (soft matter) and functional materials (hard matter).

Of current interest is the question of solid-solid interfaces, either between two misaligned domains of the same crystal structure (i.e. a grain boundary) or between two different crystal structures (polymorphs) comprised of the same constituent atoms. Predicting the stability and other properties of these interfaces is important in several contexts.

- Polycrystalline functional materials, where the performance of devices may be dominated by grain boundary (rather than bulk) properties.
- Understanding non-classical crystal nucleation and growth pathways in which crystallites with mixed polymorphic character emerge from a melt or solution.
- Predicting the mechanism of solid-solid phase transformations, where the interfacial free energy determines the longevity of metastable solids.

A particular challenge for solid-solid interfaces is constructing unit cells with which to simulate. The interfacial structure is often not known a priori, and may be spatially complex – lacking the convenient periodic symmetry exploited in bulk calculations. We will therefore concentrate on simple interfaces in the first instance.

The fcc-bcc interface is important in a number of models for nucleation and growth in soft matter. The screened-Coloumb (Yukawa) model is particularly interesting as the relative stability of the two bulk phases can be tuned. We will use advanced Monte Carlo methods to accurately compute the free energy of these interfaces and hence parameterise nucleation theories based on mixed-phase nuclei.

Another system of intense interest is ice, where very recent work has suggested that mixed nuclei of ice 1 and a previously unknown phase (ice 0) represent the first step of the freezing process. Here we will adopt global structure searching algorithms appropriate to identification of interfacial structure. We will study these in both coarse-grained and atomistic models of ice to establish if mixed-phase nuclei are thermodynamically feasible. A similar study has recently confirmed that the hexagonal and cubic polytypes of ice 1 can mix within nuclei.

Depending on the interests of the student and the outcome of funding applications in this area, further work could take a number of directions. Work on ice could be extended to study the ice 1 to ice 2 transition, recently identified as a low-pressure analogue of a solid-solid transformation implicated in triggering of deep earthquakes. We might also study the importance (or otherwise) of vibrational contributions to the stability of grain boundaries in functional ceramics, starting with well-characterised interfaces in MgO.

Students with an interest in statistical and computational physics are particularly encouraged.

7 Green, P.R.A.S. 104, 9133-9138 (2007)