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Simulation on the Edge: Modelling Surfaces and Interfaces

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Abstract

Surfaces and interfaces occur everywhere in materials science and frequently determine the properties of materials in use. Surfaces and interfaces are a multiscale problem. At the atomic scale, defects often segregate to interfaces and space-charge effects are common. Transport properties are affected both by the presence of the interface and the defects that are present. Localised electronic states are also common and even two-dimensional electron gases have been observed. For all interfaces except simple grain boundaries there is a dielectric discontinuity and therefore image effects. In hetero-epitaxial systems, stress caused by mismatch must also be considered. At the meso scale, interfaces are an essential feature of microstructures and therefore affect, and sometimes determine, the properties of polycrystalline materials.

Interfaces present a considerable challenge for simulation, particularly hetero-interfaces where the type of material is different on both sides. Examples include electrical contacts (metal and ceramic or semiconductor) and biominerals such as bones and shells (soft organic molecules or arrays and hard minerals). Interfaces often lack long-range order (and sometimes lack short-range order as well). In many problems there are different length-scales and timescales and so multiscale modelling is unavoidable.

This talk will use examples from metal/ceramic interfaces in photovoltaics, bio-interfaces and ceramic microstructures to illustrate the problems that can emerge when trying to simulate systems with interfaces. We will discuss the nucleation and growth of calcium carbonate in biological systems, contact resistance in photovoltaics and the interpretation of impedance spectra in the kinds of ferroelectric system used in capacitors.

Keywords Biominerals; Interfaces; Photovoltaics; Simulation; Surfaces