Atomistic models of reactive sputter deposition over experimental time scales

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Molecular Dynamics (MD) using reactive force field potentials has become a standard tool for investigating the first stages of low energy ion-surface interactions. However MD cannot access the time scales of experimental growth conditions because it is limited by computer power to time scales of the order of nanoseconds.

This talk will introduce a hybrid approach whereby MD is used to model the initial stages of growth, followed by an off-lattice, adaptive kinetic Monte Carlo (a-KMC) method for modelling the diffusion that occurs between particle impacts, where processes occur over longer time scales. The methodology will include a description of how to deal with events which occur rapidly in a localised region but which do not contribute to net diffusion.

A description of how the techniques can be simplified and applied to large systems using a lattice based approach while maintaining many of the a-KMC ideas will also be given.

The method will be illustrated by application to the growth of TiO₂, ZnO, Ag on ZnO and Ti on Ag [1-4] all of which are important coatings used in the glass industry. The methodology is able to identify important growth mechanisms that are non-intuitive thus giving added insight into how to optimise growth conditions.

References