Modelling nanostructure growth on a one-dimensional substrate: islands, gaps and statistics

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We study the nucleation and growth of islands during ultrathin film deposition. After the deposition of monomers or atoms onto a substrate, the nucleation and growth processes involve surface diffusion and reversible attachment to the surface and/or other monomers leading to islands formation. Islands subsequently grow either through the capture of monomers that diffuse in their corresponding capture zones or by having monomers deposited directly on them (impingement). We replicate this behaviour in kinetic Monte Carlo (kMC) simulations on a one dimensional lattice, which mimics the behaviour of monomers diffusing along a step edge, and limit our study to the scale invariant aggregation regime. We use a point island model where islands occupy a single space on the lattice and the record of their size is being incremented through the simulation. From these simulations we collect the data needed to build and test an analytic model of the system.

In an analytical description, on a one-dimensional substrate, the nucleation process translates to the fragmentation of a line into inter island gaps. Upon nucleation we describe newly created gaps by tracking the fragmentation of the old, larger one. This novel, retrospective approach gives a description of the nucleation process through Distributional Fixed Point Equations which lead to integral equations for gap and capture zone distributions. These equations belong to the broad class of Fredholm integral equations of the first kind, and they incorporate information about the critical island size and the nucleation mechanism (diffusion or impingement driven nucleation). This offers a possibility of analysing statistical data about the nucleated structures, either experimental or obtained from a simulation.

To test this model and extract more information about the system we need to solve the integral equation with no prior assumptions, with kMC data as an input. This leads us to a case of an inverse problem that is ill-posed and we use regularisation techniques to solve it.

The obtained solutions reflect different critical island sizes and fit fairly well within the expected bounds, however they also contain a high level of uncertainty due to the ill-posedness of the problem and the noise present in the input data, so further refinement of the regularisation is currently under way.

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