Modeling Strain Induced Pattern Formation and Self Organization of Quantum Dots during Heteroepitaxial Growth

C. Ratsch, X. Niu, Y.J. Lee, P. Smereka, J. DeVita, and R.E. Caflisch

It is well know that strain leads to the formation and self organization of nanostructures and quantum dots during heteroepitaxial growth. However, modeling these phenomena is a challenging task. The main reason is that elastic calculations are computationally expensive due to their long range.

In this talk, we will discuss a model for heteroepitaxial growth that we have developed in the last few years. The model employs an island dynamics model with the level-set technique in combination with a fully self-consistent elastic model. Adatoms are described in a mean-field approach, and we solve a diffusion equation for the adatom concentration. At every timestep in the simulation, we solve the elastic equations for the entire system. This is possible within our approach because the numerical timestep can be chosen much larger than in an atomistic simulation. At every lattice site strain then changes the local bonding, and thus the potential energy surface for adatoms and the microscopic parameters of the simulation. In particular, strain changes the potential energy surface for adatom diffusion, and the rate of detachment from island edges. The latter affects the boundary condition for the diffusion equation. We note that our approach includes both, the microscopic kinetic and thermodynamic driving forces that control and lead to ordering during epitaxial growth.

We will present results for several phenomena in this talk. In the submonolayer regime, we show that islands become smaller and more regular upon increasing strain, and that the island size distribution narrows and sharpens. The reason is that bigger islands are typically more strained than smaller islands, and thus their growth is slowed down. We also present results that show that strain moves the system from layer-by-layer growth to the formation of coherent islands as a mechanism for strain relieve. We will also discuss an application of our model to the growth of stacked quantum dots, where layers of islands are separated by a capping layer. Our results agree with experimentally observed trends that under the right conditions, islands nucleate above previously grown islands, and that in fact the spacing and distribution becomes more regular. Moreover, we will present results that suggest that there is an optimal thickness of the capping layer that leads to best ordering.