NANO HIGHLIGHT

Multi-scale modeling of the evolution of self-assembled quantum dots

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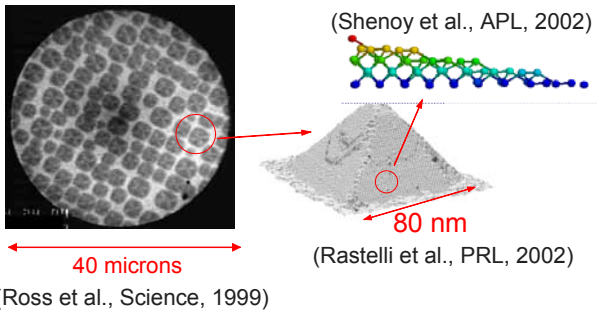
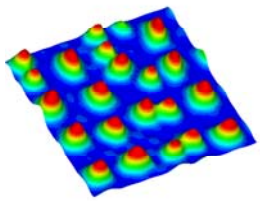
Self-organized semiconductor quantum dots hold the promise for manufacture of microelectronic devices with unprecedented performance characteristics. The quantum dots obtained by depositing SiGe alloy material on Si has been of particular interest, since they can be potentially used as memory and optical devices that are compatible with the well-developed Si technology. An example of such an array of quantum dots observed by Ross and coworkers is shown in the figure on the right. Since individual dots can be approximately 100 nm in size, each of these nanostructures comprise of hundreds of thousands of atoms. Since we are interested in analyzing periodic arrays of hundreds of such dots along with the several millions of atoms of the substrate on which these dots are deposited, simulation of structural evolution at this level of details over times significant for processing of materials provides a major challenge that is well suited to multi-scale modeling. The basic idea is to first develop quantitative understanding of phenomena that derive from the discrete nature of the material, such as atomic surface step energies and energy barriers for diffusion, by means of appropriate small-scale simulations. These "small-scale" results provide critical input to our large-scale calculations based on continuum models. This enables us to exploit our understanding of material behavior at a small size scale to explain phenomena at much larger length scales.



An example of this approach is shown in the figure on the right. The atomic structure of the stepped surface shown in the figure is based on an atomic-scale calculation of step energies. With the knowledge of the strain and orientation dependence of the surface energies from atomic scale simulations, the growth of the islands can be handled using continuum simulations. These simulations are computationally demanding due to the fact that each dot interacts with every other dot through their long-range elastic fields. We have recently developed a spectral method that speeds up the evaluation of these fields and enables simulations of large systems. The result of such a simulation is shown in the figure above. Our calculations enable us calculate a number of trends observed in experiments that were previously unexplained.



Quantum dot growth simulated
using our continuum description
(Ramasubramaniam and Shenoy, 2003)

Multi-scale modeling of quantum dot growth: The top panel shows experimental images of array of quantum dots and the shape of an individual dot along with the atomic structure that we have proposed for the sidewalls of the quantum dot. The growth of quantum dots simulated using our multi-scale approach is shown below.

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