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Simulation for Epitaxial Growth and Pattern Formation

***Russel E. Caflisch[1]**

[1] Mathematics Department, UCLA
Los Angeles, CA 90095-1555, USA
caflisch@math.ucla.edu, www.math.ucla.edu/~caflisch

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ABSTRACT

Growth of an epitaxial thin film involves physics on both atomistic and continuum length scales. In heteroepitaxial growth, e.g., Germanium on Silicon, mismatch between the lattice spacing of the Silicon substrate and the Germanium film introduces strain into the film, which can significantly influence the material structure, leading for example to the formation of quantum dots. Technological applications of quantum dot arrays require a degree of geometric uniformity that has been difficult to achieve. This talk will describe mathematical modeling, simulation methods and computational results for epitaxial growth, strain in thin films and pattern formation. The growth simulations use an island dynamics model with a level set simulation method. Strain computations can be computationally intensive, so that effective simulation of atomistic strain effects relies on an accelerated method that incorporates algebraic multigrid and an artificial boundary condition. Simulations that combine growth and strain leading to pattern formation will be presented. Applications will include lateral alloy segregation, directed self-assembly of quantum dot arrays, and vertically aligned quantum dots.