MAR05-2004-000532

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

**Simulations of Stress and Composition in Ge/Si(100) Quantum Dots**

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In this talk, I will review research, carried out in my group in recent years, on the problem of intermixing in semiconductor quantum dots (QD). The work is based on constrained-equilibrium Monte Carlo (MC) atomistic simulations, which assume that QD's are in a quasi-equilibrium state, due to the enhanced diffusion in the surface region, and which are able to address the issues of stress evolution, intermixing, and the resulting island composition. The method is applied to Ge islands grown on Si(100). Site-by-site analyses reveal inhomogeneous stress and composition profiles at typical growth temperatures, which are directly linked to each other. Comparison is made with recent experimental and other theoretical investigations. Similarities, differences, and their origin are pointed out. I present on-going efforts to include appropriate diffusion barriers in the MC algorithms, in order to examine whether some subtle differences in the theoretical and experimental profiles are of kinetic origin. I also discuss the stress evolution in the heteroepitaxial system as the islands are growing, and its association to trench formation.