565c Relaxation of Lattice-Mismatch Strain in $Si_{1-X}Ge_X$ Thin Films on Si Substrates: Modeling and Comparisons with Experiments

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Semiconductor thin films grown epitaxially on semiconductor substrates of different composition, such as $Si_{1-x}Ge_x$/Si, are becoming increasingly important in modern microelectronic technologies. In these heteroepitaxial systems, the epitaxial film is strained due to its lattice mismatch with the substrate material. Establishing process-structure-function relationships for optimizing the mechanical and electronic properties of such strained-layer heteroepitaxial systems requires development of computationally efficient models for prediction of strained-layer stability with respect to misfit dislocation formation, as well as simulation of the strain relaxation dynamics during film growth and post-growth treatment.

In this presentation, we report a hierarchical computational approach for analysis of dislocation formation, glide motion, multiplication, and annihilation in $Si_{1-x}Ge_x$ epitaxial thin films on Si substrates. The computational hierarchy includes equilibrium Monte Carlo simulations for compositional relaxation in the epitaxial film in conjunction with energy-minimization calculations for structural and strain relaxation. The above atomic-scale computations are based on rigorous, reliable many-body interatomic potentials and are combined with continuum elasticity and dislocation theory for parameterization of predictive macroscopic models for the onset of dislocation generation and the kinetics of strain relaxation. Specifically, for $Si_{1-x}Ge_x$ epitaxial thin films on Si(100) substrates, a condition is developed for determining the critical film thickness with respect to dislocation generation as a function of overall film composition, film compositional grading, and (compliant) substrate thickness. In addition, the kinetics of strain relaxation in the epitaxial film during growth or thermal annealing (including post-implantation annealing) is analyzed using a properly parameterized dislocation-mean-field theoretical model of plastic deformation dynamics due to threading dislocation loop propagation. The theoretical results are compared with experimental measurements and are used to discuss film growth and thermal processing protocols toward optimizing the mechanical response of the epitaxial film.