Order, Disorder, and Defects: Fabrication of High-Performance Semiconductor Systems

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Abstract:
Successful fabrication of nanoscale or low-dimensional semiconductors such as quantum wires and quantum dots requires an understanding of growth processes at the atomic level. First-principles density-functional calculations can be used to study the fundamental processes occurring at the surface during growth, and to provide reliable input for Monte Carlo calculations which can follow the evolution of surface over a longer time. I will report on our recent results for growth at the GaAs surface, including our explanation of the nature of the disordered “gamma phase” which is believed to approximate the steady state surface during growth under arsenic rich conditions. Successful fabrication of semiconductor devices also depends on precise control of the concentrations and locations of all electrically active defects and dopant atoms, including the native defects resulting from grown-in deviations from stoichiometry. I will discuss the recent improvements in the accuracy which can be achieved in density-functional calculations of defect properties, using as an example our work on arsenic interstitials in GaAs, which appear to play an important role in the diffusion of dopants residing on the arsenic sublattice.