Thermodynamics and Kinetics of Dislocated Ge/Si and InAs/GaAs Thin Layers

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Epitaxial layers (such as Ge/Si or InAs/GaAs) are under biaxial misfit strain, which is a strong driving force for enhanced interdiffusion. This can be a problem for heterojunction or superlattice devices. However, the misfit strain is usually fully or partially relaxed by dislocations, depending on temperature and other growth conditions. We investigate the thermodynamics and kinetics of intermixing within such dislocated thin layers through simulation and modeling. We show that appropriate injection of misfit dislocations can have the opposite effect, slowing or suppressing interdiffusion. For the simulations we use the continuous-space Monte Carlo method, employing multi-component empirical potentials. The thermodynamic and kinetic models employed rely on a parameterization of the free energy in terms of the elastic energy as given by the linear theory of elasticity.

The results for Ge/Si(001) show a significant reduction in the rate of interdiffusion in the presence of dislocations, leading to substantially less alloyed quantum wells. Note, that the ideal non-dislocated superlattice becomes throughout a random alloy at thermodynamic equilibrium. In the case of the InAs/GaAs(001) superlattice the suppression of interdiffusion in the InAs layer is even more pronounced. This can be explained by the substantially different lattice mismatch between the constituent layers (4% and 7%, respectively). The composition profiles resulting from the semi-analytic thermodynamic model are in agreement with the simulations and aid in the understanding of the underlying physics: in the region between the interfaces the enhanced strain relaxation provided by the dislocations minimizes the elastic energy and reduces entropic mixing.

In actual experimental conditions the thermodynamic equilibrium might be unreachable due to the presence of dislocation-enhanced kinetic barriers in the diffusion process. We provide a measurement of these barriers both through simulation and modeling, thus illustrating the possibility of using dislocations in order to critically damp intermixing.