Lateral alloy segregation in thin heteroepitaxial films

CHRISTIAN RATSCH, JASON REICH, XIAOBIN NIU, YOUNGJU LEE, RUSSEL CAFLISCH, UCLA — We have studied the segregation and alloy formation of thin heteroepitaxial films. We use an atomistic strain model that has a cubic geometry and includes nearest neighbor bonds, next nearest neighbor bonds, and bond bending terms. Our motivation is the well established fact that for many heteroepitaxial systems growth proceeds in the Stranski-Krastanov growth mode, where islands form after the formation of a wetting layer. Recent results indicate that intermixing and thus vertical variations of the alloy concentration are a crucial factor in controlling the formation and thickness of the wetting layer. Our results suggest that in addition to vertical segregation there is also lateral segregation. Thermodynamically, the system prefers to have one big feature of the epilayer material that is embedded in the substrate but is near the surface. In practise, there will be a typical separation distance of these features because of kinetic limitations. We postulate that this lateral segregation and the separation of these features is ultimately responsible for the lateral placement of islands on the surface.