The Atomic-Scale Mechanisms of Ternary Semiconductor Alloy Growth: Self-limited vs. Accumulating Anion Processes

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Alloys of compound semiconductors are necessary to create heterostructures for optoelectronic and electronic devices. Growth of alloys that vary the cation component, eg: AlGaAs or InGaP, is fairly straight forward because there are few reactions between the cation species. Growth of mixed anion alloys, such as InAsSb and GaSbBi, are more complex because of the strong tendency for the individual anion species to interact. In the case of InAsSb, for instance, the displacement of Sb with impinging As is well documented. Furthemore, it is proposed that Sb atoms are weakly physisorbed on the surface. We investigate this hypothesis by scanning tunneling microscopy coupled with *ab initio* total energy calculations. We show that rather than remaining weakly physisorbed, Sb roughens the surface by increasing the coverage of divots (vacancy clusters) and two dimensional islands. Our calculations show how that As-terminated surface reconstructions may transform into mixed heterodimer terminated configurations, which causes the roughening by pulling atoms from the terrace. Thus we propose an alternative model for interfacial broadening by intermixing rather than by surface segregation. Another example of a complex mixed anion alloy is the Bi-containing materials system. The growth of GaAsBi and GaSbBi often leads to low Bi incorporation, droplets on the surface, and nonuniformity in the composition. We have developed a kinetic Monte Carlo simulation that explicitly takes cation and anion reactions into account that is capable of examining the unique characteristics of Bi-containing III-V semiconductor alloys. A phase diagram for a range of growth rates was generated using this simulation that predicts both Bi content and droplet formation. Furthermore, we propose a new kinetic model that captures the dynamics of incorporation and droplet formation in the growth of these alloys.

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