Reconstruction and Disorder at Compound Semiconductor Surfaces

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Compound III-V semiconductor surfaces reconstruct to minimize dangling bonds and surface free energy. The specific atomic structure of the reconstruction is determined by a number of competing factors, including local chemical bonding and long range electrostatic and strain interactions. In alloys, these long-range interactions can induce coexistence of different reconstructions and can couple surface reconstruction domains to the morphology and compositional non-uniformity of the grown material. At typical growth temperatures, surface disorder and the associated configurational and vibrational entropy also have a strong influence on the observed surface structure. In collaboration between the DOE Center for Integrated Nanotechnologies (CINT) and the University of Michigan, we have been developing computational tools to help achieve a quantitative understanding of surface structure and nanostructure formation at semiconductor alloy surfaces. In order to help determine the atomistic structures of experimentally observed surface reconstructions, we have developed an algorithm that systematically enumerates all possible structures of a specified symmetry consistent with a widely applicable set of rules. Building on the resulting structures, we have coupled density functional theory calculations, the cluster expansion approach, and Monte Carlo methods to address the effects of the disorder associated with alloying and finite-temperature on surface reconstruction.

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