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Numerical simulations of VLS heteroepitaxial nanowire growth

VIVEK SHENOY, Brown University, KLAUS SCHWARZ, JERRY TERSOFF, IBM T. J. Watson Center — Nanowires are particularly attractive for designing heterostructures, as effective radial strain relaxation allows heterostructures with a wider range of material combinations. The electrical, optical, and thermal properties of the nanowire are highly dependent on the accurate control of the locations and thicknesses of such heterostructures. However, in the case of nanowire growth from a metal seed particle, the composition of the seed particle will vary for growth of different materials due to alloying, which may cause problems in controlling interface abruptness. Also, recent experiments have shown that in many cases, growth instabilities do not allow for the formation of nanowires with desired morphology and material combinations. We have developed a continuum model for the growth of heteroepitaxial nanowires, and we use it to study the factors that control interface abruptness and instabilities during growth. Our model includes the following features that are critical for capturing the composition profiles in nanowires: 1) the differences of the attachment rates of the alloy components at the catalyst-wire interface, 2) the possibility of a miscibility gap in the alloy phases of the catalyst and the nanowire, 3) composition dependence of the surface energies of the nanowire and nanowire-catalyst interface and 4) anisotropy in surface energies leading to faceted morphologies.

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