Mechanisms of Morphological Evolution on Faceted Core-Shell Nanowire Surfaces

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Core-shell nanowires with radial heterostructures hold great promise in photonic and electronic applications and controlling the formation of these heterostructures in the core-shell configuration remains a challenge. Recently, GaAs nanowires have been used as substrates to create AlGaAs shells. The deposition of the AlGaAs layer leads to the spontaneous formation of Al-rich stripes along certain crystallographic directions and quantum dots near the apexes of the shell. A general two-dimensional model has been developed for the motion of the faceted solid-vapor interfaces for pure materials that accounts for capillarity and deposition. With this model, the growth processes and morphological evolution of shells of nanowires around hexagonal cores (six small facets {112} in the corners of six equivalent facets {110}) are investigated in detail both analytically and numerically. It is found that deposition can yield facets that are not present on the Wulff shape. These small facets can have slowly time-varying sizes that can lead to stripe structures and quantum dots depending on the balances between diffusion and deposition. The effects of deposition rates and polarity (or asymmetry) on planes {112} on the development of the configurations of nanowires are discussed. The numerical results are compared with experimental results giving almost quantitative agreement, despite the fact that only pure materials are treated herein whereas the experiments deal with alloys.