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Theoretical Analysis of Equilibrium Surface Segregation in Ternary III-V and II-VI Semiconductor Nanostructures SUMEET PANDEY, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present an atomic-scale analysis of equilibrium surface segregation in ternary compound (III-V and II-VI) semiconductor nanostructures. The analysis is based on a computational scheme for compositional and structural relaxation that combines Monte Carlo with conjugate-gradient methods according to properly modified/extended parameterizations of the valence-force-field (VFF) description; the VFF parameterizations employed in the analysis are validated by comparison with first-principles density functional theory calculations. We report equilibrium concentration distributions in slabs of $In_xGa_{1-x}As$ and $ZnSe_{1-x}S_x$ as a function of composition, x, slab thickness, and slab surface crystallographic orientation, as well as in $In_xGa_{1-x}As$ and $ZnSe_{1-x}S_x$ nanocrystals with well-defined surface facets as a function of x and nanocrystal size. The results are discussed in the context of synthesis of core/shell structures of ternary compound semiconductor nanocrystals for increased quantum-dot photoluminescence efficiency.

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