Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Compositional Distribution in Semiconductor Ternary Quantum Dots and Its Effects on Their Optoelectronic Properties XU HAN, University of Massachusetts-Amherst, SUMEET PANDEY, Micron Technology Inc., DIMITRIOS MAROUDAS, University of Massachusetts-Amherst — We present a systematic theoretical and computational analysis of compositional distribution in semiconductor ternary quantum dots (TQDs) and the resulting effects on the TQDs' electronic band structure. The analysis is based on a hierarchical modeling approach that combines first-principles density functional theory calculations and classical Monte Carlo simulations with a continuum model of species transport in spherical nanocrystals. In many cases of TQD composition, the model predicts the formation of core/shell-like structures characterized by the formation of concentration boundary layers near the nanocrystal surfaces. A systematic analysis over the size-composition parameter space generates a database of transport properties that is used to design post-growth thermal annealing processes to establish thermodynamically stable compositional distributions in TQDs. We explore the impact of compositional distribution on the TQDs' electronic band gaps and find that TQDs with thermodynamically stable compositional distributions allow for precise band-gap tuning. Our findings lead to a proposal for an efficient one-step TQD synthesis method followed by annealing to promote self assembly of the thermodynamically stable configuration, for optimal optoelectronic function in devices.

Xu Han
University of Massachusetts-Amherst

Date submitted: 07 Nov 2012 Electronic form version 1.4