Morphology of Cu$_2$S-CdS and Ag$_2$S-CdS Nanorod Heterostructures

DENIS DEMCHENKO, Virginia Commonwealth University, BRYCE SADTLER, University of California, Berkeley, HAIMEI ZHENG, A. PAUL ALIVISATOS, LIN-WANG WANG, Lawrence Berkeley National Laboratory — A partial cation exchange has been used to synthesize Cu$_2$S-CdS and Ag$_2$S-CdS nanocrystal heterostructures, with two very different morphologies. Cu$^+$ cation exchange takes place preferentially at the ends of CdS nanorods, Cu$_2$S segments grow into the nanorod from both ends. Ag$^+$ exchange is non-selective, Ag$_2$S islands nucleate and grow over the entire surface of the nanorod. This leads to very different patterns, striped Ag$_2$S-CdS superlattice with several equidistant Ag$_2$S segments in a CdS nanorod, and an asymmetric Cu$_2$S-Cds heterostructure with Cu$_2$S segments at the ends of the CdS nanorod. We use first-principles calculations to obtain formation energies of the different epitaxial interfaces between Cu(Ag)$_2$S and different facets of CdS nanorods. Comparison of chemical and elastic contributions to the interface formation energy for the Cu(Ag)$_2$S-CdS shows that the relative stability of the interfaces determines the nucleation of Cu(Ag)$_2$S and the resulting morphology. Furthermore, since two end facets of CdS nanorod are not crystallographically equivalent a controlled asymmetric nucleation of Cu$_2$S can occur.

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