

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Morphology of Cu_2S -CdS and Ag_2S -CdS Nanorod Heterostructures¹ 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_2S -CdS and Ag_2S -CdS nanocrystal heterostructures, with two very different morphologies. Cu^+ cation exchange takes place preferentially at the ends of CdS nanorods, Cu_2S segments grow into the nanorod from both ends. Ag^+ exchange is non-selective, Ag_2S islands nucleate and grow over the entire surface of the nanorod. This leads to very different patterns, striped Ag_2S -CdS superlattice with several equidistant Ag_2S segments in a CdS nanorod, and an asymmetric Cu_2S -CdS heterostructure with Cu_2S segments at the ends of the CdS nanorod. We use first-principles calculations to obtain formation energies of the different epitaxial interfaces between $\text{Cu}(\text{Ag})_2\text{S}$ and different facets of CdS nanorods. Comparison of chemical and elastic contributions to the interface formation energy for the $\text{Cu}(\text{Ag})_2\text{S}$ -CdS shows that the relative stability of the interfaces determines the nucleation of $\text{Cu}(\text{Ag})_2\text{S}$ and the resulting morphology. Furthermore, since two end facets of CdS nanorod are not crystallographically equivalent a controlled asymmetric nucleation of Cu_2S can occur.

¹Supported by U.S. DOE, DE-AC02-05CH11231 and NERSC.

Denis Demchenko
Virginia Commonwealth University

Date submitted: 21 Nov 2008

Electronic form version 1.4