136c Relative Stability and Morphology of Si Nanowires [Invited]

A. Tchernatinsky, D.B. Migas, C. Leahy, M. Yu, C.S. Jayanthi, and S.Y. Wu

The morphology and relative stability of silicon nanowires oriented along <001>-, <011>-, <111>-, and <112>-direction have been studied using density functional theory- and semiempirical Hamiltonian-based molycular dynamics (MD) schemes. The diameter of the nanowires considered ranges from 2 to 15 nm. We find that Wulff construction is applicable for the determination of the shape of the nanowire. In addition, facets as well as edges between facets on the surface are crucial factors in optimizing the shape of the nanowire. Our finding indicates that, for diameters in the range of <10 nm, silicon nanwires oriented along <011>-direction display the lowest total energy, consistent with recent experimental observations.