Electronic Phase Diagram of Single-Element Silicon “Strain”
Superlattices\textsuperscript{1} ZHENG LIU, University of Utah, WENHUI DUAN, JIAN WU, Tsinghua University, MAX LAGALLY, University of Wisconsin-Madison, FENG LIU, University of Utah — The evidence that the band gap of Si changes significantly with strain suggests that by alternating regions of strained and unstrained Si one creates a single-element electronic heterojunction superlattice (SL), with the carrier confinement defined by strain rather than by the chemical differences in conventional compositional SLs. Using first-principles calculations, we map out the electronic phase diagram of a one-dimensional pure-silicon SL. It exhibits a high level of phase tunability, e.g., tuning from type I to type II. Our theory rationalizes a recent observation of a strain SL in a Si nanowire and provides general guidance for the fabrication of single-element strain SLs.

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