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Bandstructure Effects in Unstructured AlGaAs Nanowires
NEERAV KHARCHE, CLEMENS HEITZINGER, GERHARD KLIMECK, Purdue University, MATHIEU LUISIER, ETH Zurich, Switzerland, TIMOTHY BOYKIN, Univ. Alabama in Huntsville — Atomic scale alloy disorders can have profound effects on the bandstructure and charge transport through nanowires. With decreasing diameters down to nanometer scales, alloy disorder can no longer be treated in an average manner using the virtual crystal approximation (VCA). Our zone unfolding algorithm along with supercell calculations can be used to treat alloy disorders even to atomic scales. We calculate bandstructures and transmission coefficients of AlGaAs random alloy nanowires with diameters ranging from 2nm to 6nm. Using the nanoelectronic modeling tool (NEMO3D), eigenstates of the alloy nanowire supercell are calculated with the 20-band sp3d5s* spin model. Small cell bandstructures are then projected out of the supercell eigenstates. Transmission coefficients are calculated with an atomistic NEGF simulation of the alloy wire embedded between two ideal reservoirs. These projected bandstructures and transmission coefficients both show reduced bandgaps and noisy behavior and provide significant insight into the physics of charge transport.

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