Effects of Electronic and Strain Boundary Conditions in Multi-million Atom Electronic Structure Simulations

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NEMO 3-D is a Nanoelectronic Modeling Tool, which enables the electronic structure simulation of arbitrarily shaped zincblende semiconductor structures that include up to 32 million atoms. The empirical tight binding model using s, p, and d orbitals is optimized using a genetic algorithm to fit experimental bulk properties and employed to as a basis set for the representation of nanometer-scale objects. Self-assembled InGaAs quantum dots grown on GaAs are subject to significant variations in the local strain distribution. An accurate calculation of the electronic structure requires an accurate representation of the positions of each atom since the orbital couplings also depend on the relative positions of the nearest neighbor atoms, an. NEMO-3D uses a valence force field model to minimize the total strain energy, expressed as a sum of local (nearest-neighbor) functionals of atomic positions. Different electronic (open and periodic) and strain (fixed, open, and periodic) boundary conditions can be employed in NEMO 3-D. Results employing these different boundary conditions applied to the finite simulation domain will be discussed for binary InAs as well as alloyed InGaAs quantum dots will be discussed. The dependence of the eigenenergy level and the alloy disorder noise as a function of embedding GaAs buffer size will be discussed in particular.