Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems

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Nonatomistic models such as **k.p** are often used to characterize the electronic structures of quantum dots. However, such jellium-like models are fundamentally not well suited for the atomistic representation of nanoscale features such as interfaces and disorder. We are currently developing an atomistic nanoelectronic simulation tool (NEMO-3D) to model quantum dot structures on high performance commodity clusters (Beowulfs). Modeling of realistic structures entails simulation domains encompassing many millions of atoms. Such large-scale domains result in very large eigenproblems (dimension $\gtrsim 10^8$) which necessitate the usage of massively parallel computers. The first part of the work will address the numerical issues that need to be (and have been) tackled to deal with such a large problem. Scaling results will be presented that illustrate the performance of our algorithm on a Beowulf commodity cluster. On dual CPU Pentium III systems the performance of the two CPUs is significantly reduced if large memory blocks exceeding 500MB are accessed by each CPU. The performance reduction may be so severe that it may be more advantageous, to leave one CPU idle and let the other CPU operate on 1GB RAM.

Our simulation employs a nearest-neighbor tight-binding model ($sp^3d^5s^*$) with a 20 orbital basis, consisting of s, p, and d orbitals, associated with each atomic lattice site. Since the basis set that is used is not complete in a physical sense, the parameters that enter the model do not correspond precisely to actual orbital overlaps. Thus, an analytical approach to determine these parameters is insufficient. Instead, a genetic algorithm package is used to determine a set of orbital couplings that reproduce a large number of physical observables of the bulk binary system, including bandgaps and effective masses at various symmetry points in the Brillouin zone. These orbital couplings must also depend on bond lengths to account for the shifts in atomic positions in strained systems. A power-law scaling is assumed (whose exponent is also determined with the genetic algorithm) to account for strain-induced shifts. Since an accurate calculation of the electronic structure within the tight-binding model also necessitates an accurate representation of the positions of each atom, NEMO-3D uses a valence force field (VFF) model in which the total strain energy, expressed as a local (nearest-neighbor) functional of atomic positions, is minimized.

In this work, we demonstrate results that arise from this atomistic representation that cannot be obtained through simple effective mass approximations. First, we demonstrate that calculations for low lying eigenstates on "identical" (i.e same size) quantum dots that vary only in the distribution of cation species are shown to display noticable spatial variations in the electron eigenstates and very large variations in the hole eigenstates (see figure). The greater localization of the hole eigenfunctions arises from the larger hole mass which has a lower binding energy and is therefore more sensitive to local perturbations. Second, the distribution of ground state electron and hole energies is shown to be roughly Gaussian with a spread of several meV. Two sources of disorder contribute to this spread – a compositional disorder, which arises from random configurations of cations subject to a constraint of fixed numbers of cations of each species, and a concentrational disorder stemming from random variations in the number of cations. It is found that the contribution of concentrational disorder to the broadening of the ground state eigenenergies dominates on all length scales up to several million atoms.

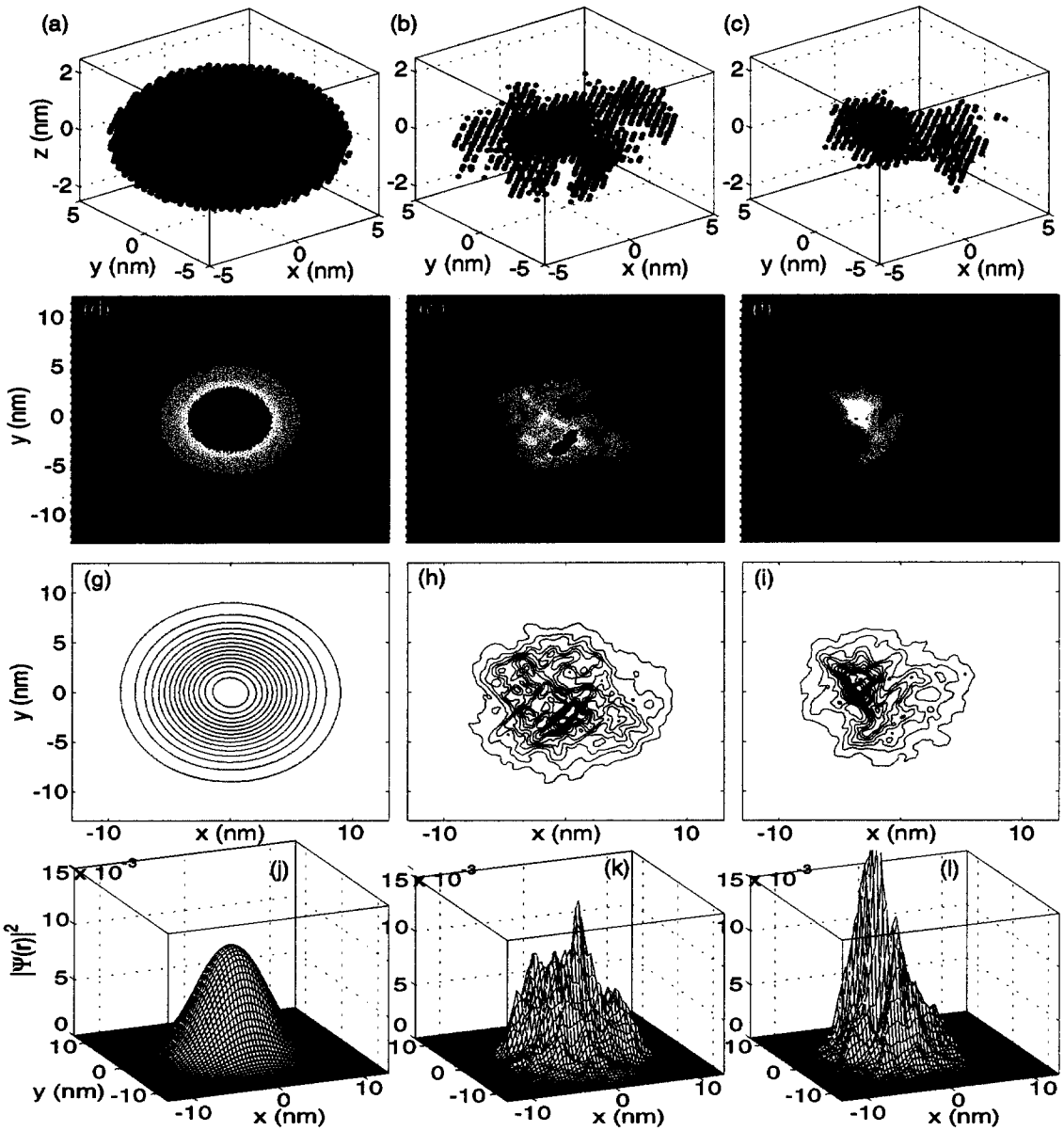

Figure 1: Comparison of hole ground state wave functions for a lens-shaped $In_{0.6}Ga_{0.4}As$ dot of diameter 30 nm and height 5 nm embedded in a GaAs buffer containing approximately 3 million atoms for several cases – a dot composed of an "artificial" homogeneous VCA material (first column), and two different random configurations (middle and right column). First row: scatter plot of wavefunction in 3-D. Second, third, and fourth row: colored contour plot, outlined contour and surface plot sliced at z=0 nm, respectively.