Atomistic Simulation of Quantum Dots Including Strain and Bandstructure and Full Band Simulation of Hole Transport in 1-D Heterostructures.

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As microelectronic research moves devices to nanometer scale operating at GHz speeds, the physics of electron flow through devices becomes more complicated and physical effects, which previously could be ignored safely in microelectronic devices, become significant. High energy electron injection, quantization of charge, quantization of energy, electron-electron, electron-photon and other electron scattering interactions are some of the phenomena that are presently being investigated experimentally and theoretically. Raytheon/TI developed a 1-D quantum device simulator (NEMO-1D) to address such issues. In 1-D heterostructures In that effort expertise in device physics, numerical and graphical user interface technologies were combined to produce the first quantitative, general-purpose quantum device simulator. The work presented here is an extension of the of the NEMO 1-D software to massively parallel high performance computing to enable the simulation of hole transport and to 3-D modeling to enable quantum dot simulations.

NASA's interest in long wavelength infrared imaging and the advancements of computation technology has sparked research in quantum dots at JPL. Near term interest in self-assembled InAs quantum dots on GaAs substrates lies in far-infrared detectors with reduced dark current, increased temperature of operation, increased radiation hardness, and increased sensitivity over quantum well infrared detectors. Long term interest in quantum dots is induced by their potential use as computational units in future computer architectures.

Since the InAs quantum dots are highly strained in the GaAs matrix it is essential to model the effects of this strain on the electronic structure. We have recently implemented a nearest neighbor tight binding model including s, p and d orbitals that can model conduction and valence bands *throughout the Brillouin zone*. This model, unlike its sibling the second-nearest neighbor sp3s*, can include effects due to stress and strain in a straight forward way, since it is only based on two-center orbital integrals. The large number of orbital interaction energies in this model are fit to experimentally observed quantities such as bandgaps, effective masses, and strain induced shifts using a genetic algorithm package [1]. The mechanical strain in the quantum dots is computed via conjugate gradient-based minimization using the Keating potential [2]. Resonance states are computed using a customized parallel Lanczos eigenvalue solver for systems of about one million atoms.

InSb-based inter band cascade lasers are good candidates for future far infrared lasers. They include the tunneling of hole into electron states. We started our study hole of transport in a simpler system where experimental data on hole transport is readily available: a hole resonant tunneling diode in GaAs/AlAs. Heterostructures such as resonant tunneling diodes break the symmetry of the crystalline lattice. Such break in lattice symmetry can cause a strong interaction of heavy-, light- and split-off hole bands. This strong interaction results in a complicated transverse subband dispersion. This work demonstrates that it is essential to include this transverse subband dispersion into current computation via explicit integration over the transverse momentum. The Tsu-Esaki approximation which work reasonably well for electron transport is shown to completely break down for hole transport. It is found that the dominant current contribution stems in wide bias ranges from holes that are traveling through the structure with non-zero transverse momentum (off the Γ zone center). The transverse subband dispersion causes the semiconductor to act like an indirect bandgap material for holes. Parallelization of the numerical energy and momentum integrals in the NEMO-1D simulation tool were required to undertake these simulations since the current flow is dominated by very sharp resonance linewidths (10^{-8} eV) in a large energy range that are non-local and sharply peaked in k-space.

[1] G. Klimeck, et al, accepted in Superlattices and Microstructures (2000).
[2] P. Keating, Phys. Rev. v.145, p.637, (1966).

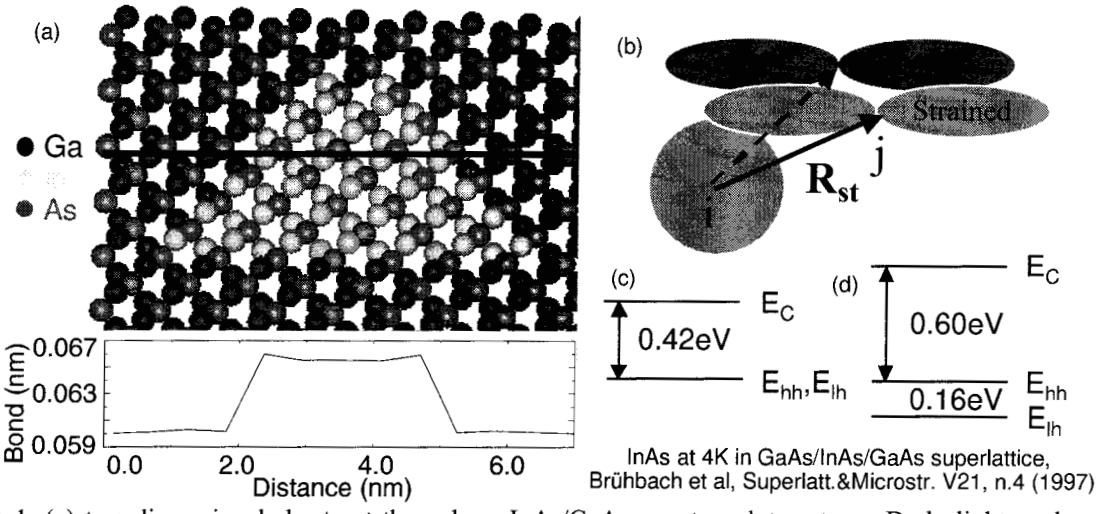

Figure 1: (a) two-dimensional sheet cut through an InAs/GaAs quantum dot system. Dark, light, and gray dots indicate Ga, In, and As atoms, resptectively. Black horizontal line indicates approximate cut in which the bond length between atoms is depicted below. The strained bond length is calculated with the Keating potential. (b) Sketch of effect of atomic repositioning due to strain in a orbital point of view. Overlaps between the various orbitals can change dramatically due to strain. (c) unstrained InAs bandgap. (d) Experimental data of strained InAs bandgap from cited reference.

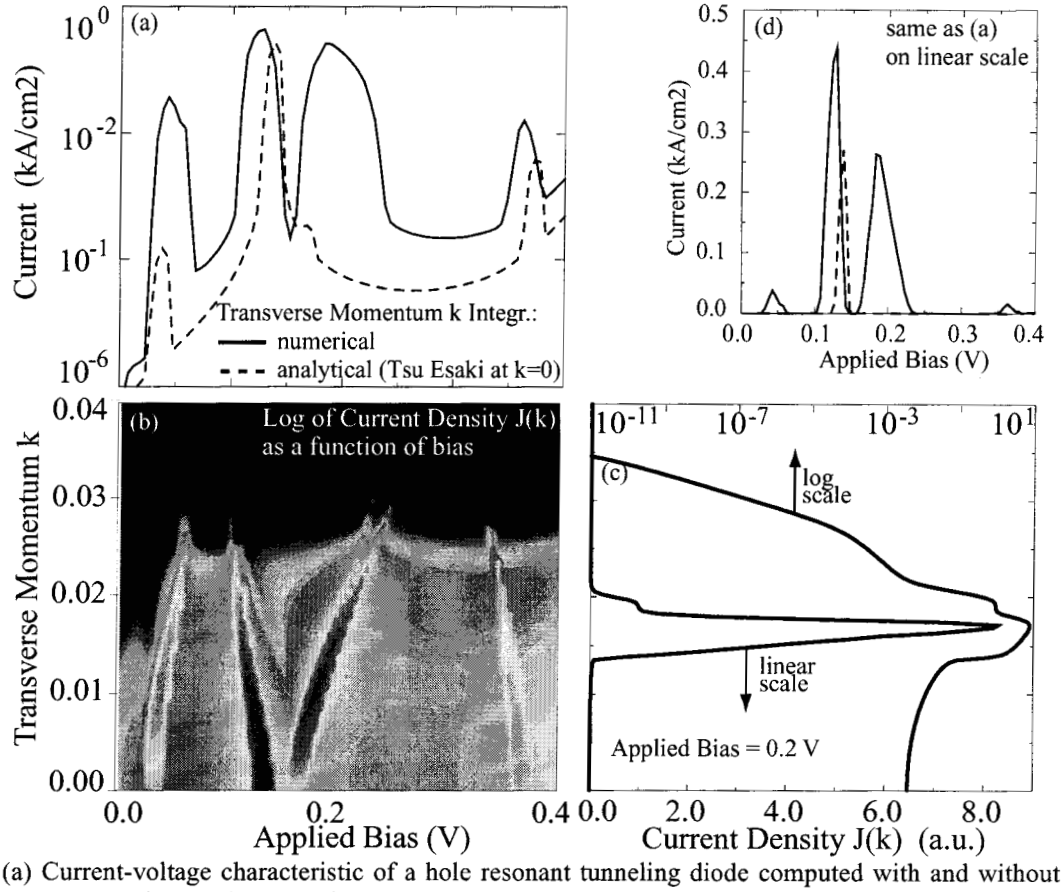

Figure 2: (a) Current-voltage characteristic of a hole resonant tunneling diode computed with and without explicit transverse momentum integration. Dashed curve corresponds to a cut through (b) at k=0. (b) Integrand current density J(k) as a function of transverse momentum and bias. Gray scale ranges from dark, over light back to dark. Almost vertical streaks indicate large current density along a pattern similar to the subband dispersion E(k) (c) Cut through (b) at a voltage of 0.2V on a linear and logarithmic scale. The most significant current contribution occurs at about k=0.018 off the zone center at k=0. (d) same as (a) on a linear scale. Full band integration in energy E and transverse momentum k is essential to capture all hole transport channels in a hole resonant tunneling diode.