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1D hetero-structure tool for atomistic simulation of nano-devices

Samarth Agarwal
Purdue University - Main Campus

Kaushik Balamukundhan
Purdue University - Main Campus

Neophytos Neophytou
Purdue University - Main Campus

Gerhard Klimeck
Purdue University - Main Campus, gekco@purdue.edu

1D hetero-structure tool for atomistic simulation of nano-devices.

Samarth Agarwal[1,2],Kaushik Balamukundhan[2],Neophytos Neophytou[2] and Gerhard Klimeck[2]
[1]Department of Physics, Purdue University, West Lafayette, IN-47907
[2]Network for Computational Nanotechnology, Birck Nanotechnology Center,
Purdue University, West Lafayette, IN-47907

Abstract

Quantum mechanical effects are becoming increasingly important in realistic devices as their critical sizes reduce to a few nanometers. Equally important, yet not really appreciated is the ability to capture the details at the atomic level to capture effects of band-to-band mixing, band-non-parabolicities, and crystal orientations. The 1D hetero-structure tool presented here is based on the nearest neighbor tight-binding model (sp^3d^5s*) that naturally captures these effects. The Non-equilibrium Green's Function approach is used for transport calculations, in addition to the computation of electronic structure using a combination of numerical methods. Both open boundary conditions for arbitrary crystallographic orientations and closed boundary conditions can be applied. A sophisticated energy grid generation technology is employed that reduces simulation time and ensures that features are accurately captured without excessive compute times. The capabilities of the interactive simulator which will be deployed on nanoHUB.org are demonstrated.

Introduction and approach

It has been recognized for several years now, that effective mass models are inadequate to capture crucial details in devices with material variations at atomic dimensions. In addition to that a quantum-mechanical approach is necessary to explain the effects of geometry and band-structure. Here we use the sp^3d^5s* tight binding model to capture band-structure effects in 1D hetero-structures and demonstrate the capability of a simulator capable of handling various geometries in various materials. The model has been chosen since the s and p orbitals are enough to model the valence bands, and the excited d orbitals are necessary to model the conduction band over the entire Brillouin zone and to include the correct strain scaling behavior. In addition to that spin-orbit coupling is essential to get the correct valence bands.[2]

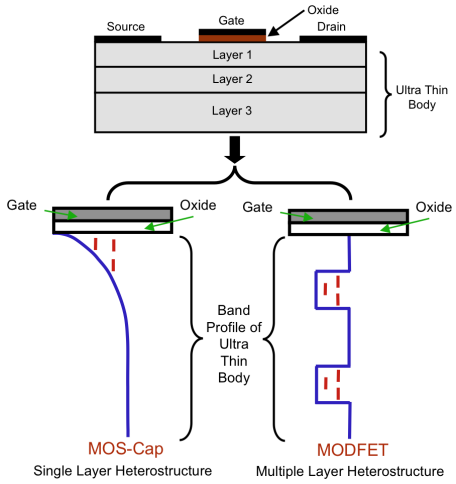
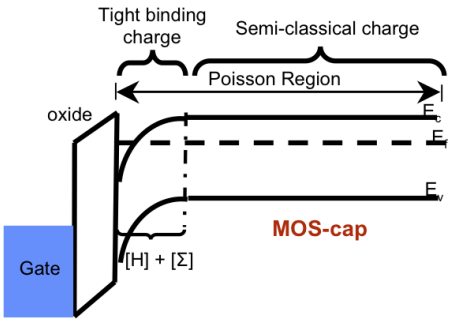
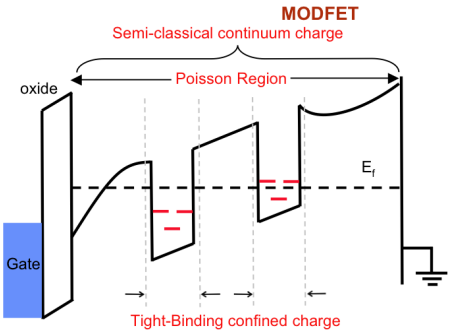


Figure 1: Schematic drawing of a UTB

Fig.1 shows schematically the kind of devices we are interested in modeling. The gate to substrate direction is the crystal growth direction which can be controlled at the atomic level. Compared to this direction where ma-



(a)



(b)

Figure 2: Simulation domains of (a) MOS-CAP and (b) MODFET

terial variations can happen on the nanometer scale with atomic layer precision, the lateral directions are extremely large. We consider them infinite and apply periodic boundary conditions. In charge calculations the use of closed boundary conditions[3] implies that the wave-function should decay at the boundary, while using open boundary conditions[4] allow an exchange of wavefunction probability with the contacts. Within the generalized simulator set-up dramatically different devices and materials can be considered such as a MOS-Capacitor(Fig.2a) or a Modulation Doped FET(Fig.2b). In either device there is distinction between regions where it is necessary to calculate charge quantum mechanically and where it is sufficient to calculate charge semi-classically using a Thomas-Fermi model. The distinction comes from the presence of discrete confined states as opposed to a continuum of states.

MOS-CAPs

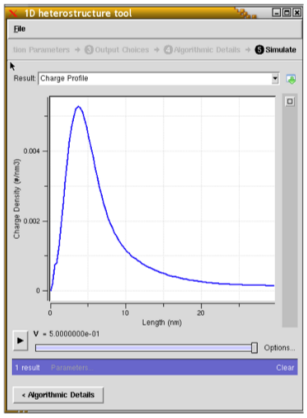


Figure 3: MOS-CAP Charge profile

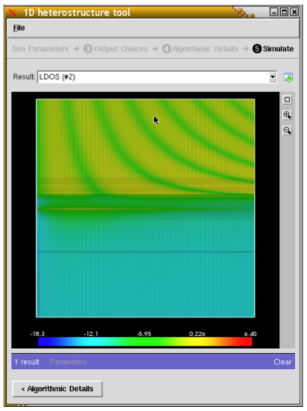


Figure 4: MOS-CAP Density of States

Fig.3 shows the charge as a function of distance in the device, of a GaAs MOS-Capacitor. The charge is calculated using the density of states obtained from the Green's Function technique. The levels are populated using a Fermi level determined by the doping in the substrate. Since the gate is present on the left side we use closed boundary conditions such that the wave-function dies out. On the right side we use open boundary conditions to model the flat band conditions in the substrate. The density of states plot (Fig.4) shows confined states lying inside the triangular potential well. Features in the density of states above the confined states

can also be seen, as waves piling against the semi-conductor oxide barrier, which is a signature of continuum states injected from the open boundary on the right. Outside the tight binding region it is sufficient to calculate the charge semi-classically since there are no confined states. Finally all the charge calculation has to be done self-consistently with the electrostatic potential which accounts for the free and movable charge. We model the oxide at the oxide semi-conductor interface as a region with a linear drop of potential since we assume that there is no charge inside the oxide. On the substrate side we let the potential approach flat band conditions.

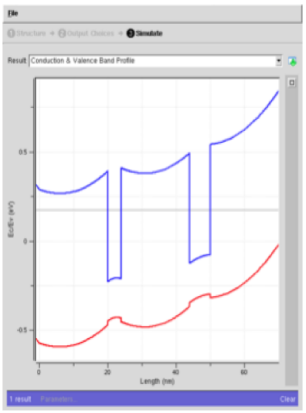


Figure 6: MODFET Band Profile

Quantum Wells

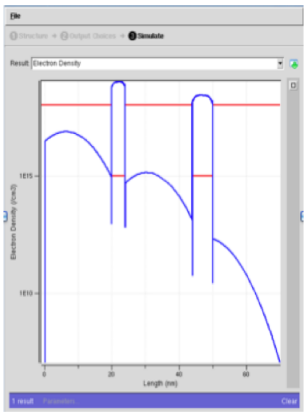


Figure 5: MODFET Charge Profile

As an example of the modeling capabilities of heterostructures we present the results for an $Al_xIn_{1-x}Sb$ based Modulation Doped FET device. It can be seen from the charge profile(Fig.5) and the band profile(Fig.6) that close to the quantum wells, charge has contributions from both confined as well as continuum states. The charge in this case is calculated semi-classically outside the wells. Charge in the confined states for each well is calculated by constructing a Hamiltonian using the well material with closed boundary conditions on both sides. The bandstructure of the geometry is then calculated based on the eigenvalues of the Hamiltonian. The eigen-vectors give the spatial variation of charge inside the wells. The eigenvalues in this case are real as opposed to the case when we use open boundary conditions. In the case of open boundary conditions the eigenvalues are complex, where the imaginary part corresponds to the lifetime of the state. The quantum mechanically computed charge replaces the charge which was previously computed semi-classically. These calculations are done self-consistently with the electrostatic potential.

Tool features

To accurately capture the physical quantities in the device at a reasonable computational cost, a number of numerical techniques have been used in the simulator(Fig.7). To integrate over the density of states an adaptive energy grid generation technique is used. The technique allows the addition of energy nodes in the integration range where the integrand varies rapidly. This is achieved by successive partitioning. This insures that integration nodes are only added as required to achieve a certain level of accuracy. If the resonances are weakly coupled to continuum reservoir states, their lifetime may be extremely long, resulting in energetically very sharp resonances. It may be extremely expensive to resolve these resonances through adaptive refinement. We therefore also imple-

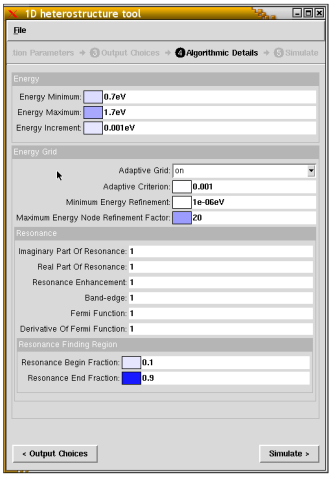


Figure 7: Tool Input options:Algorithmic Details

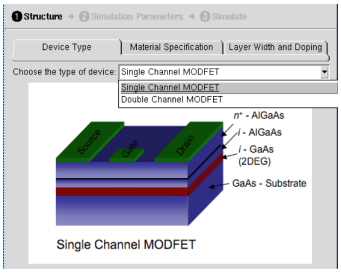


Figure 8: Tool Input options: Device geometry

mented a resonance finder, which determines the eigen-energy and the lifetime or width of the state and therefore allows for the resolution of the resonances with very few energy nodes. The problem of finding resonances is non-linear because of energy dependent open boundary conditions. The idea is to find good starting guess values to resonances using Shift and invert non-symmetric Lanczos[1], for the Newton technique to locate the values accurately. The simulator gives the user access to a large material database based on effective mass and the sp^3d^5s* model. The user can design the device in great detail. Fig.9 shows the various dimensions necessary to make a Modulation Doped FET. In addition to that the doping profile inside the device can also be specified.

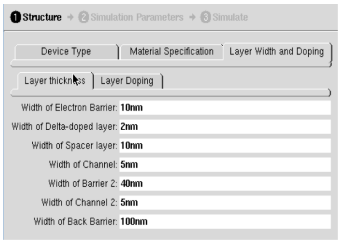


Figure 9: Tool Input options: Geometry details

Conclusions

Here we have demonstrated a 1D heterostructure simulation tool based on the sp^3d^5s* tight binding model, that should prove beneficial to experimentalists and theoreticians alike. The tool will be deployed on nanoHUB.org

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