# Planar Supercell Simulations of 3D Quantum Transport in Semiconductor Nanostructures

D. Z.-Y. Ting, S. K. Kirby, and T. C. McGill

Thomas J. Watson, Sr., Laboratory of Applied Physics California Institute of Technology Pasadena, California 91125, U.S.A.

### Abstract

We introduce the planar supercell method as a means for treating 3D quantum transport in mesoscopic tunnel structures. The flexibility of the method allows us to examine a variety of physical phenomena relevant to quantum transport, including alloy disorder, interface roughness, defect impurities, and 0D, 1D, and 2D quantum confinement, in device geometries ranging from double barrier heterostructures to quantum wire electron waveguides. As examples, we examined quantum transport in double barrier structures with interface roughness, and in quantum wire electron waveguides.

## I. Introduction

In modeling quantum transport in semiconductor resonant tunneling heterostructures, one can often assume perfect periodicity in the lateral directions, thereby reducing the mathematical description to a 1D problem in which only the potential variation along the growth direction need be considered. However, in realistic device structures we need to take into account imperfections such as interface roughness, impurities, and alloy disorder which are incompatible with the assumption of translational invariance in the parallel directions. In this work, we introduce the planar supercell method as a general purpose model for treating these structural imperfections. The model is designed for flexibility so that it can be used not only to study tunnel structures such as the double barrier heterostructure, but also lower dimensional mesoscopic devices such as quantum wire electron waveguides. Using this method, we have studied how the transport properties of double barrier heterostructures are influenced by interface roughness. We also briefly report on a study of transport in quantum wire electron waveguides.

#### II. Method

We use a planar supercell tight-binding Hamiltonian and specify a structure as a stack of  $N_z$  layers perpendicular to the z-direction, with each layer containing a periodic array of rectangular planar supercells of  $N_x \times N_y$  sites. Within each planar supercell, the potential assumes lateral variations as dictated by the device geometry. Figure 1 illustrates a set of planar supercell stacks used in simulating double barrier structures with interface roughness. Our model is formally equivalent to the one-band effective mass equation[1]

$$-\frac{\hbar^2}{2}\nabla \cdot \frac{1}{m(\mathbf{x})}\nabla\psi + V(\mathbf{x})\psi = E\psi,$$
(1)

discretized over a Cartesian grid, and subject to periodic boundary conditions (with su-

percell periodicity) in the x- and y-directions, and open boundary conditions in the zdirection. The transmission coefficients for structures described by the planar supercell stack can be determined by the direct application of the multiband method developed by Ting et al. [2]



Fig. 1. A set of planar supercell stacks used in simulating double barrier structures with interface roughness. Light and dark areas represent sites occupied by well and barrier materials, respectively. Cross sections shown are the  $25 \times 16$  planar supercells representing the rough interfacial layers between the quantum well and the second barrier. Note that the supercells are repeated in the lateral directions.

## **III.** Applications

To illustrate the applications of the planar supercell method, we examine the effect of interface roughness on transmission properties of double barrier structures, and effects of neutrl impurities and geometric imperfections in quantum wire electron waveguides.

#### Interface Roughness

Figure 2 shows transmission spectra near the n = 1 resonance for a set of GaAs/AlAs double barriers structures with interface roughness as depicted in Figure 1. For each GaAs-AlAs interface on the incident side, a 50% random coverage rough interfacial layer is placed between the pure GaAs layers and the pure AlAs layers. Random configurations of interfacial layers with different island sizes are generated with a simulated annealing

algorithm.[3] Three of the structures have average island sizes ( $\lambda$ ) of 28 Å, 49 Å, and 106 Å; an additional reference structure with smooth virtual crystal approximation (VCA) Al<sub>0.5</sub>Ga<sub>0.5</sub>As alloy interfacial layers is included for comparison. We note that the spectra for structures with rough interfaces show a series of satellite peaks not present in the reference structure spectrum. The satellite peak strength increases with island size, but peak positions are approximately the same for all three rough structures. The satellite peaks are the result of interface roughness induced k<sub>||</sub> scattering of off-resonance states into on-resonance states. In principle, interface roughness can scatter a given k<sub>||</sub> into a continuous range of k'<sub>||</sub>. But due to the finite supercell size, k<sub>||</sub> can scatter only into a discrete set of  $N_x \times N_y$  parallel k vectors differing from it by a reciprocal lattice vector. Therefore the contributions from the scattered states appear as individual satellite peaks. The spacing between satellite peaks can be decreased with larger supercell sizes. For sufficiently large supercells, the spacings would become smaller than the resonance peak width, and the satellite peaks would then coalesce.



Fig. 2. Transmission coefficients for a set of GaAs/AlAs double barrier structures with rough interfaces as depicted in Fig. 1.

Fig. 3. Transmission coefficients for structures similar to those shown in Fig. 2, except that the island sizes are larger.

0.21

The scattering mechanism described above accounts for how interface roughness can reduce peak-to-valley ratios in current-voltage characteristics of double barrier resonant tunneling diodes by increasing off-resonance transmission coefficients. The other major effect of interface roughness is the broadening of resonance peaks through wave function localization. In Figure 3 we show transmission spectra for a set of structures similar to those in the previous example, but with larger island sizes of 112 Å, 304 Å, and 424 Å.

We note that the n = 1 transmission resonance down-shifts and broadens with increasing island size. This can be explained in terms of wave function localization. The presence of the rough interfacial layer between the quantum well and the second barrier introduces well width fluctuation, and in effect divides the structure into wide-well ( $L_W = 13$ , in this example) and narrow-well  $(L_W = 12)$  regions. If the island sizes are sufficiently large (compared to the de Broglie wavelength), it is possible to have quantum well states whose wave functions are laterally localized in the wide-well regions. Since the wide-well regions are also the narrow-barrier regions (second barrier width of  $L_B = 4$  rather than 5), the transmission resonance associated with these localized states should be down-shifted (due to the wider well), and broadened (due to the narrower barrier).



Fig. 4. Transmission coefficients for a set of quantum wire electron waveguide with different waveguide opening geometries.

Fig. 5. Transmission coefficients a set of quantum wire electron waveguide with and without neutral impurity.

0.40

0.45

#### **Electron Waveguide**

We explore the transmission properties of quantum wire electron waveguides with the planar superscell method. Using discretization sizes of  $d_x = d_y = d_z = 5 \text{\AA}$  and  $16 \times 16$ planar supercells, we modeled a GaAs quantum wire structure 200Å in length,  $40Å \times 40Å$ in cross section, surrounded on the sides by AlAs walls, and the ends by GaAs electrodes. To study the sensitivity of transport properties to waveguide opening geometry, we have modeled two similar structures. The first has slightly wider waveguide openings : at the two ends of the waveguide, the cross section is widened to  $60 \text{\AA} \times 60 \text{\AA}$  for the first 5 Å (lengthwise), and  $50\text{\AA} \times 50\text{\AA}$  for the next 5 Å; the rest of the wire remains  $40\text{\AA} \times 40\text{\AA}$  in cross section. The other structure is obtained by simply capping the ends of the original

structure with 15 Å thick AlAs layers. Figure 4 shows the transmission spectra for the three structures described above. We see that the amplitude of the transmission coefficients and the resonance positions and widths vary considerably in these structures.

In the final example we study the effect of neutral impurities on transport properties of electron waveguides. We model three waveguide structures : one with no impurities, another with an attractive impurity at the center of the waveguide, and a third with an impurity near the waveguide opening. Figure 5 provides a picture of how an impurity perturbs the waveguide transmission spectrum. We note that an impurity near the waveguide opening does not strongly perturb the lowest two resonances since these modes have small probability densities near the waveguide opening. However, an impurity at the waveguide center down-shifts and narrows the lowest (n=1) resonance while leaving the n=2 mode relatively unperturbed. (Note that the n=3 mode has also been down-shifted to near the n=2 resonance.) This is because the n=1 resonance has the largest probability density at the center of the waveguide, while the n=2 mode has a node at the center.

## **IV.** Summary

We discussed the planar supercell method as a means for treating 3D quantum transport in mesoscopic tunnel structures. We demonstrated its applications with studies of interface roughness in double barrier heterostructures, and geometric imperfections in electron waveguides. In addition to the examples discussed here, we have also use our method to study the effect of alloy disorder and impurity scattering in various device geometries. We found the flexibility of the method to be extremely useful in exploring a wide range of issues relevant to the operation of tunnel devices.

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