Three-Dimensional Quantum Transport by Supercell Method: Numerical Acceleration and Applications

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Summary

The open-boundary planar supercell stack method treats three-dimensional quantum transport in mesoscopic tunnel structures in a numerically stable and efficient manner. We formulate quantum mechanical scattering problems for supercell geometry as sparse linear systems, and solve them by iterative methods. Recent improvement in solution algorithm using a seven-diagonal pre-conditioner has resulted in over two orders of magnitude of numerical acceleration, bringing more flexibility in the range of problems we can tackle. We will discuss applications to interface roughness in double barrier resonant tunneling structures, tunneling characteristics of ultra-thin oxides undergoing dielectric breakdown, and quantum well infrared photodetectors.

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The exactly solvable, real-space, open-boundary planar supercell stack method (OPSSM) has been applied to a variety of topics involving 3D quantum transport in mesoscopic devices [1]. OPSSM formulates quantum mechanical scattering problems for supercell geometries as sparse non-Hermitian linear systems, and solve them iteratively by the Quasi-Minimal Residual (QMR) method [2]. The convergence rate of the QMR method can be greatly accelerated with appropriate pre-conditioning. Figs. 1 and 2 illustrates performance gains achieved using a 7-diagonal pre-conditioner in typical applications involving MOS tunnel structures and GaAs/AlAs double barrier structures. With over two orders of magnitude of numerical acceleration (see Table 1), we are now able to obtain more accurate results by using larger supercells. Fig. 3 illustrates that supercell periodic boundary condition induced artifacts in the transmission coefficient spectrum of a double barrier structure with interface roughness [3] are reduced significantly with the use of larger supercells. The flexibility of the method has enabled us to include elastic scattering effects due to impurities, interface roughness, and alloy disorder in our studies of 2D (double barrier heterostructures), 1D (quantum wires electron waveguides), and 0D (quantum dots) mesoscopic device structures. As examples, we will discussion results on studies of interface roughness effects and dielectric breakdown in n^+ poly-Si/SiO$_2$/p-Si tunnel structures containing ultra-thin oxide layers [4, 5]. We will also discuss recently applications to the studies of intersubband infrared detectors.

Table 1. Speed-up obtained in typical 3D scattering calculations with a 7-diagonal pre-conditioner.

	No Pre-conditioner	7-Diagonal Preconditioner	Speed-Up
DBH 16x16x26	8.92 h	1.66 h	5.4
DBH 32x32x26	208.7 h	17.6 h	12
DBH 64x64x26	1511 h (Poor Convergence)	283.2 h (Good Convergence)	>> 5
MOS 64x64x37 (Tol=1E-10)	1618.5 h	23.2 h	70
MOS 64x64x37	1618.5 h (Tol=1E-10)	5.7 h (Tol=1E-7)	284

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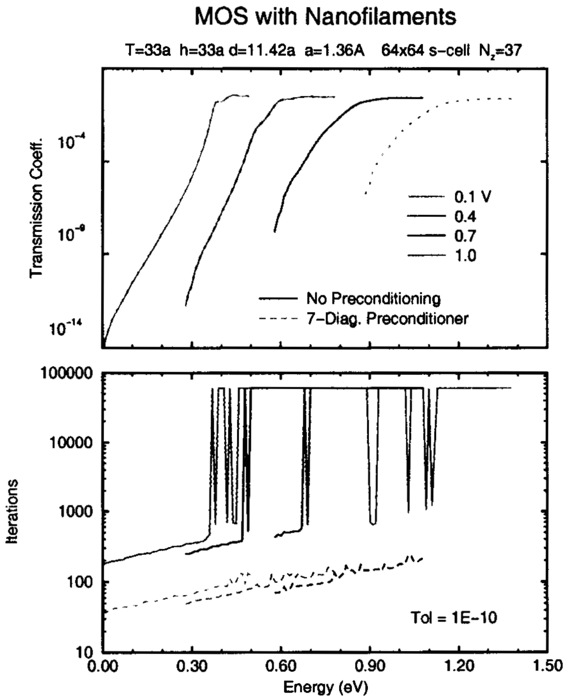

Figure 1. Upper panel shows transmission coefficient spectra of an ultra-thin oxide layer embedded with nano-filaments under several biasing conditions. Lower panel shows convergence iterations counts with and without the 7-diagonal pre-conditioner

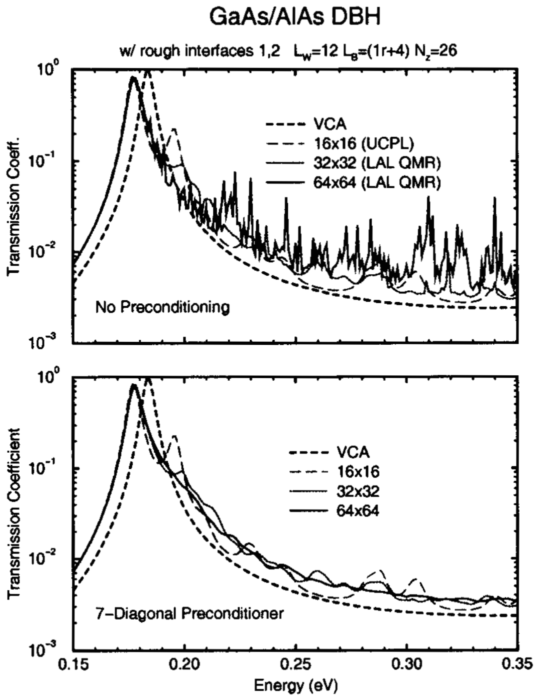

Figure 3. Transmission coefficient spectra of GaAs/AlAs double barrier structure computed using various supercell sizes. Numerical accelation by pre-conditioning made large supercell calculations possible, thus enabling the reduction of artifacts due to supercell-periodic scattering.

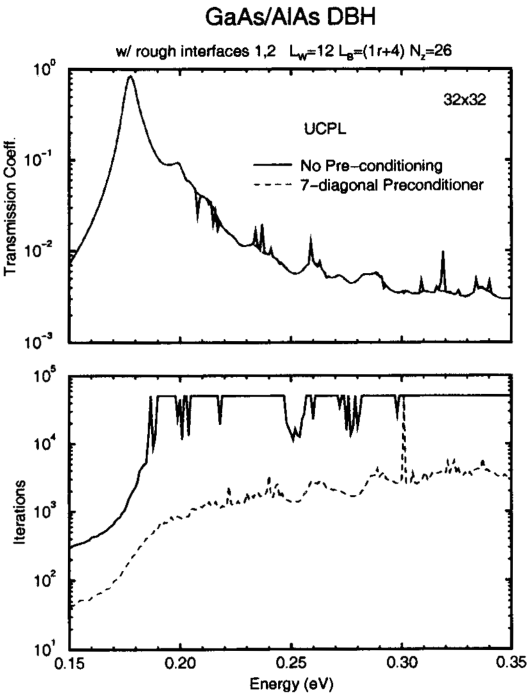

Figure 2. Upper panel shows transmission coefficient spectra of GaAs/AlAs double barrier structure. Lower panel shows convergence iterations counts with and without the 7-diagonal pre-conditioner. A limit of 50,000 iteration is used.

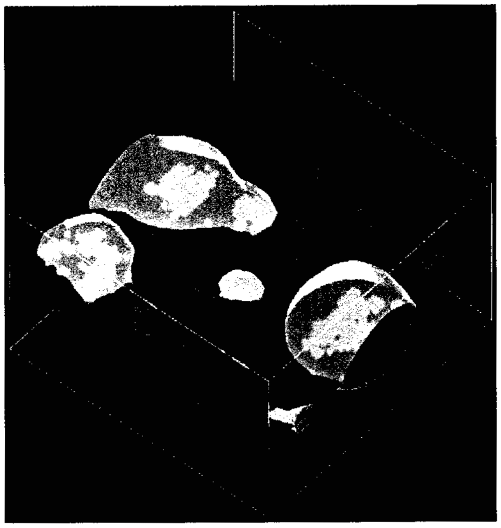

Figure 4. A probability density isosurface (white translucent surfaces) for the lowest resonance in a GaAs/AlGaAs double barrier structure with 1/6 monolayer of InAs embedded in mid-well. Solid-colored cross sections of the structure showing the double barrier structure and the mid-well layer are also shown. The insertion of the InAs fractional monolayer introduces lateral variations in the envelope function, and can modify intersubband absorption characteristics of quantum wells.