Numerical Approximations for Polar Optical Phonon Scattering in Resonant Tunneling Diodes

Gerhard Klimeck, Roger Lake, Chenjing L. Fernando, R. Chris Bowen, Daniel Blanks, Manhua Leng*, Ted Moise, Y. C. Kao and William R. Frensley*

Corporate R&D, Texas Instruments Incorporated, Dallas, TX 75235
**School of Engineering, University of Texas at Dallas, Richardson, TX 75083*

Polar optical phonon scattering (POP) strongly controls the the valley current in many types of resonant tunneling diodes (RTDs). To facilitate RTD device design we have developed a general purpose quantum device simulator (NEMO) that provides numerous modeling options for 1-D confined structures. Based on the non-equilibrium Green function formalism we evaluate numerical approximations for the polar optical phonon interaction self-energies (full matrix, tridiagonal matrix, diagonal matrix, and omission of the real part) by comparing current densities, electron densities and overall current-voltage (I–V) characteristics. A scaled diagonal matrix treatment of POP scattering is found to be sufficient to mimic full matrix polar optical phonons. Simulations including POP scattering and interface roughness scattering are compared directly to experimental data. The calculated valley current agrees to within 10% of the experimental data for the modeled device.

Resonant tunneling diodes may provide the best opportunity for near term applications of quantum effect devices. Two of the major impediments of circuit applications of RTDs are: 1) their significant current flow in the off-state (valley current) and 2) their large sensitivity to layer thickness and doping profiles. Simulation tools are needed to explore the design space of high performance RTDs. Design tools can help the engineer to minimize RTD valley currents and their sensitivity to process fluctuations. We have designed and implemented a general purpose 1-D quantum device simulator, NEMO (Nanotechnology Engineering MOdeling tool), that provides the versatility of an interactive design tool and a comprehensive analysis tool. NEMO offers several models for quantum charge self-consistency, bandstructure models and scattering, and it offers several levels of approximation for treating each model. The approximations trade off computation time and physical detail. In this paper we demonstrate and discuss the range of validity for several approximations to the polar-optical-phonon scattering self-energy.

The inclusion of scattering in quantum transport simulations is computationally and memory intensive. Without scattering, the calculation of the current and electron density formally requires the calculation of the first and last columns of the inverse of a tridiagonal matrix, $(E-H_0)$, in a single-band tight-binding representation, where H_0 is the bare Hamiltonian. With polar-optical-phonon

scattering, the calculation of the current and electron density requires the calculation of the first and the last column of the inverse of a full matrix, $(E-H_0-\Sigma)$, where the full matrix, Σ, is the self-energy resulting from polar-optical-phonon scattering. A recursive Green function algorithm[1] used for a partial inversion of the $N \times N$ tridiagonal matrix scales linearly as N. The partial inversion of the $N \times N$ full matrix scales as N^2. To utilize the favorable scaling of computation time and memory of tridiagonal systems, we have implemented two approximations of the full matrix treatment of the POP self-energies: truncation of the full matrix to a 1) tridiagonal matrix or 2) diagonal matrix.

While the inclusion of scattering alone is computationally and memory intensive, including the effect of scattering in a fully self-consistent calculation of the electro-static potential can be numerically almost prohibitive. The self-energies distort and shift the resonance spectrum of the quantum system which can significantly affect the calculation of the charge density. We will show that by ignoring the real part of the self-energies, the spectrum shift is minimized, the fully self-consistent calculation can be avoided, and the simulation results still agree well with the experiment.

The peak-to-valley ratio of RTDs is ultimately determined by scattering in the best devices. The scattering mechanisms that give rise to valley currents in RTDs have been studied using a number of different approaches.[2–5] Our approach is based on the non-equilibrium Green function formalism.[6] The effect of scattering is included through self-energy terms in a truncated self-consistent Born type approximation.[7] This algorithm is similar to the multiple sequential scattering algorithm described by Roblin and Liou.[4] We model interface roughness as a single layer of alloy where the cations of a single species cluster into islands.[8] The standard bulk Fröhlich Hamiltonian[9] is used to model the POP interaction. Since the self-energies have a strong momentum dependence, we numerically integrate over the incident transverse momenta.

We compare our I–V simulations with the experimentally measured I–V obtained from a GaAs-AlAs RTD with 19.5 nm intrinsic GaAs spacer layers, 3.1 nm AlAs barriers, and a 6.2 nm GaAs well. The n^+ contacts are Si doped at 10^{18} cm^{-3}. Measurements are made at a temperature of 4.2 K to eliminate tunneling through X states in the AlAs barriers. Figure (1) shows the measured I–V and simulations with and without scattering. The experimental curve shows a weak shoulder in the voltage range of 0.38–0.5 V, which is called the phonon peak. The electrostatic potential is obtained from a self-consistent Schrödinger-Poisson calculation including a local density approximation for the exchange-correlation terms[10] but excluding the effects of scattering. This potential is also used for the simulation of the current which includes the effect of scattering. This approach was also used in references [3, 4]. In Figure (1) we set the real

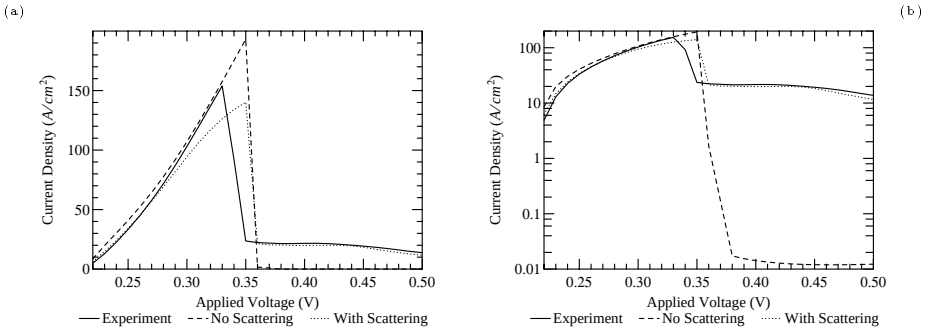

Figure 1: (a) I–V measured at 4.2 K (solid line), simulated without scattering (dashed line) and with scattering (dotted line) from polar optical phonons and interface roughness (correlation length 10 nm). (b) Same as (a) on a logarithmic scale.

part of the scattering self-energies, Σ, due to polar optical phonons and interface roughness (IR) to zero for reasons discussed following Figure (4). The full polar optical phonon self-energy matrix is approximated as diagonal in the results shown in Fig. (1) with a scaled coupling strength.

Figure (1) shows that while the scattering-free calculation provides a sufficient estimate for the peak current and the peak voltage, it underestimates the valley current by three orders of magnitude. The valley current is dominated by incoherent scattering. We now discuss the modeling of the valley current in detail and focus first on the modeling of POP without IR scattering.

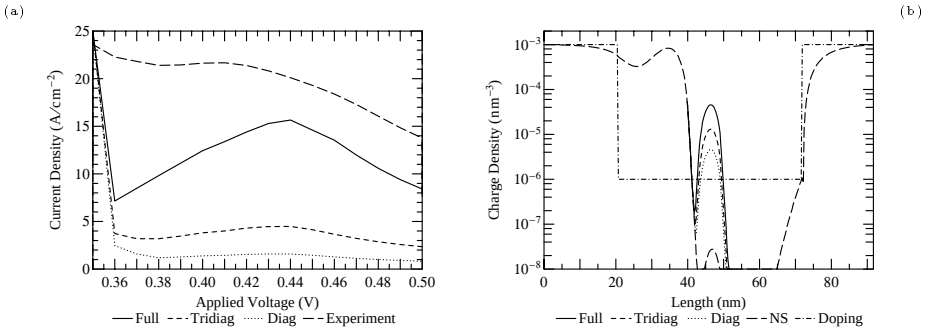

Figure 2: (a) Valley current calculated for three different POP models: full matrix (solid line), tridiagonal matrix (dashed line), and diagonal matrix (dotted line), and experimental data (long dashed line). (b) Well electron density calculated in the three models of (a) at a bias of 0.44 V. The electron density calculated without scattering (NS) and the doping profile are shown as well.

Figure (2a) shows the valley current calculated for three different POP models without IR scattering co-plotted with the experimental data. The real part

of the scattering self-energies, Σ, is included. The tridiagonal and the diagonal approximation of the POP self-energy predict a smaller current than the full matrix calculation, by factors of 3.1–3.7 and 8.3–10.6, respectively. Also, the calculated electron density is reduced by about the same factors, as shown for a single bias voltage of 0.44 V in Figure (2b). We conclude from this example that a simple truncation of the full POP self-energy to a tridiagonal or diagonal matrix significantly underestimates the POP interaction. Note that even the full matrix treatment underestimates the measured valley current (we will address this mismatch further below).

Given the results of Figure (2), the question arises as to whether the diagonal and tridiagonal matrix approximations can be useful. We explore the scaling of the diagonal matrix approximation to mimic the full matrix result. The scaling is performed by a simple multiplicative increase of the POP interaction strength. Figure (3a) depicts the valley current calculated in the diagonal matrix approximation for scaling factors of 1, 4, 8, and 12 compared to the full matrix result. A factor of 12 calculated in the diagonal matrix approximates the valley current calculated in the full matrix approach well. The deviation from the full matrix result is at most 10%. Figure (3b) demonstrates for one bias point (0.44 V) that the well electron density is scaled correctly by a scaling factor of 12 as well. For that particular bias point the deviation is less than 3%.

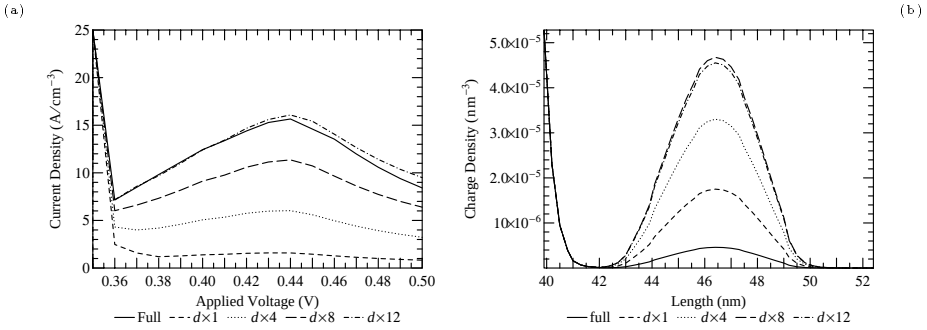

Figure 3: (a) Valley current calculated for the diagonal matrix approximation for different scaling factors of 1 (short dashed line), 4 (dotted line), 8 (dashed line) and 12 (dashed-dotted line) compared to the full matrix result (solid line). (b) Quantum well electron density which was calculated in the different models of (a) at a bias of 0.44 V.

The scaling constant used to increase the POP scattering strength in the diagonal matrix approximation is structure dependent. For other GaAs-AlGaAs structures that we have examined at low temperatures in our single band analysis, a constant in the range of 10–12 provides good results. The addition of a "free" scaling parameter is rewarded by a reduced memory requirement and

reduced computation time. For this example the full matrix approach required 89 MB of RAM and 180 minutes of computation time on a single CPU of a Silicon Graphics Powerchallenge (MIPS R8000) for each bias point. The diagonal matrix approximation required 35 MB of RAM and took 6 minutes. The memory requirement was reduced by a factor of 2.5 and CPU time was reduced by a factor of 30, while the calculated I–V deviates at most 10%. The scaling parameter can be tuned at a single bias point in the valley with all other scattering mechanisms turned off. The reduced computation time pays off especially, if other scattering parameters like the interface roughness correlation length are to be varied in a set of numerical experiments or if a fully self-consistent potential calculation is desired.

Polar optical phonon scattering alone is insufficient to explain the valley current as shown in Figure (2). In Figure (4a), experimental data are compared to simulations which includes POP scattering (diagonal model, scaling factor of 12) and interface roughness (IR) scattering. The IR is characterized by a 10 nm island size and modeled with an exponential correlation function.[8] Neither scattering mechanism alone can make up for the experimentally measured valley current, however both scattering mechanisms together match the valley current within 10%.

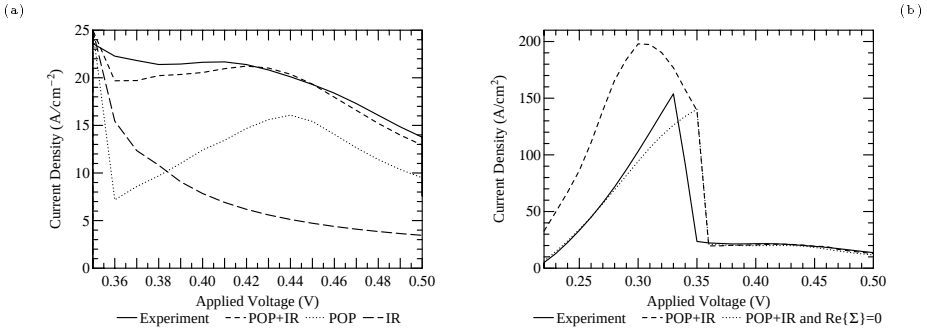

Figure 4: (a) Experimental I–V (solid line) and valley current calculated for POP scattering alone in the diagonal approximation scaled by a factor of 12 (dotted line), interface roughness (IR) alone with a exponential correlation model and an correlation length of 10 nm (long dashed line) and POP and IR together (dashed line). (b) Experimental I–V (solid line) and simulations including both, POP and IR (dashed and dotted line). Ignoring the real parts of Σ (dotted line) does not alter the valley current significantly, but maintains the shape of the main resonance peak.

Figure (4b) compares the overall I–V curve to experimental data. The simulation including IR and POP matches the valley current to within 10%; however, the peak current is distorted. The distortion of the peak current results from two

things, the shift and distortion of the resonant spectral lineshape by the real part of the self-energy[8] combined with an electrostatic potential that is not calculated self-consistently with the changed spectrum. Preliminary calculations indicate that a fully self-consistent calculation of the electrostatic potential which includes the effects of the scattering self-energies removes the distortion. To avoid the computational requirements of such a fully self-consistent electrostatic potential calculation, NEMO gives the user the option of ignoring the real part of the self-energy. This generally gives good agreement with experiment.

In summary, we have presented the substitution of a diagonal matrix for the full matrix treatment of POP scattering. The charge and current densities calculated within the scaled diagonal matrix approximation are within 10% of the full matrix calculation. This approximation decreases the required CPU time by a factor of 30 and the required memory by a factor of 2.5 in the current version of NEMO. This dramatic increase in simulation throughput provides an essential stepping stone towards a fully self-consistent potential calculation that includes scattering-assisted charging effects. Alternatively, one can ignore the real part of the self-energies for a faster but more approximate solution. The simulations including polar optical phonon scattering and interface roughness scattering showed agreement with experiment to within 10% in the valley current region. Using NEMO, we have been able to match the current in a GaAs-AlAs RTD. We believe that such a predictive tool used for the exploration of the rich RTD design space is necessary to bring quantum devices to practical circuit application.

References

[1] R. Haydock, in *The Recursive Solution of the Schrödinger Equation*, Vol. 35 of *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1980), p. 215.

[2] The references [3-5] and their citations provide a good overview of the literature.

[3] F. Chevoir and B. Vinter, Phys. Rev. B **47**, 7260 (1993).

[4] P. Roblin and W. Liou, Phys. Rev. B **46**, 2416 (1993).

[5] R. Lake and S. Datta, Phys. Rev. B **45**, 6670 (1992).

[6] S. Datta, in *Electronic Transport in Mesoscopic Systems or Current Flow in Small Conductors*, edited by H. Ahmed, M. Pepper, and A. Broers (Cambridge University Press, New York, 1994), and references herein.

[7] R. Lake, G. Klimeck, R. C. Bowen, and D. Jovanovic, submitted to J. Appl. Phys. (1996).

[8] R. Lake *et al.*, accepted for publ. in Superlattices and Microstructures (1996).

[9] H. Fröhlich, Proc. Roy. Soc. London, Ser. A **160**, 230 (1937).

[10] E. Gawlinski, T. Dzurak, and R. A. Tahir-Kheli, J. Appl. Phys. **72**, 3562 (1992).