Documentation of the 3D NEGF–SCBA Simulator for a GaAs/AlAs Resonant Tunneling Diode with Doping-Dependent Fermi Level

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1 Overview

This document provides a detailed explanation of a three-dimensional (3D) to one-dimensional (1D) reduced non-equilibrium Green's function (NEGF) simulation for a GaAs/AlAs double-barrier resonant tunneling diode (RTD). The simulator includes localized inelastic scattering through the self-consistent Born approximation (SCBA) and accounts for transverse modes, coherent background current, and a defect-induced phonon-assisted tunneling channel.

The updated version of the simulator incorporates a **doping-dependent Fermi level**, computed using degenerate semiconductor statistics rather than being specified directly as an input. This ensures physical consistency with real highly-doped GaAs emitters/collectors.

2 Device Geometry and Material Stack

The simulated device consists of the following symmetric heterostructure:

GaAs (8 nm) / AlAs (1.5 nm) / GaAs (2 nm) / AlAs (1.5 nm) / GaAs (8 nm)

GaAs serves as emitter and collector, while the 2 nm GaAs quantum well hosts the resonant state(s). AlAs forms two 1.5 nm barriers.

Effective masses and band edges:

- $m^*_{\mathrm{GaAs}} = 0.067 m_0$
- $m^*_{\mathrm{AlAs}} = 0.15 m_0$
- Conduction band offset: $E_c^{\mathrm{AlAs}} - E_c^{\mathrm{GaAs}} = 0.57$ eV

A finite-difference discretization with spacing $a_0 = 0.12$ nm is used to build the 1D Hamiltonian H_0.

3 Doping and Fermi Level Calculation

In the updated simulator, the Fermi level is not a free parameter. Instead, the user provides a donor concentration N_D (in cm^{-3}), which is converted to m^{-3} and used to compute $E_F - E_C$ from:

$$n = \frac{2}{\sqrt{\pi}} N_C F_{1/2}\left(\eta_F\right), \qquad \eta_F = \frac{E_F - E_C}{kT},$$

where N_C is the effective density of states and $F_{1/2}$ is the Fermi–Dirac integral.

We numerically invert this expression (using Brent root-finding) to obtain the physically correct Fermi level for degenerately doped GaAs. This ensures:

- correct occupation of states,
- a physically consistent left/right chemical potential under bias,
- correct selection of transverse modes.

During the bias sweep:

$$\mu_L = E_F + \frac{qV}{2}, \qquad \mu_R = E_F - \frac{qV}{2}.$$

4 NEGF Framework

The effective longitudinal energy is:

$$E_{\text{eff}} = E - E_\perp.$$

For each $(E, E_\perp)$ pair, the retarded Green's function is:

$$G^r(E) = \left[(E + i\eta)I - H_0 - \Sigma_L - \Sigma_R - \Sigma^r_{\text{inel}}\right]^{-1}.$$

4.1 Contact Self-Energies

Using 1D tight-binding semi-infinite leads:

$$\Sigma_{\text{lead}} = t_0 e^{ika}, \qquad k = \arccos\left(\frac{E - U}{2t_0}\right).$$

5 Transverse Mode Integration

The total current density is obtained by integrating over transverse energy:

$$J = \frac{2q}{h} \int D_{2D}(E_\perp) I(E_\perp)\, dE_\perp,$$

where the 2D density of states

$$D_{2D} = \frac{m^*}{\pi\hbar^2}$$

is constant for parabolic bands.

6 Localized Inelastic Scattering via SCBA

A single site in the middle of the well is treated as a localized phonon/odorant defect, with:

$$\hbar\omega = 36 \text{ meV}, \qquad D^2 = (8 \text{ meV})^2.$$

The SCBA equations are:

$$\Sigma^{<}_{\text{inel}}(E) = D^2\Big[(N_{ph}+1)G^{<}(E+\hbar\omega) + N_{ph}G^{<}(E-\hbar\omega)\Big], \tag{1}$$

$$\Sigma^{>}_{\text{inel}}(E) = D^2\Big[N_{ph}G^{>}(E+\hbar\omega) + (N_{ph}+1)G^{>}(E-\hbar\omega)\Big], \tag{2}$$

applied only at the defect site, with iterative updates until convergence.

7 Mode Selection Criterion

Only transverse modes that satisfy *both* inequalities are treated inelastically:

$$E_\perp > E_C^{\text{left}}, \qquad E_\perp < \mu_L - (E_F + \hbar\omega),$$

ensuring that the longitudinal energy window supports phonon-assisted emission.

Modes outside this window contribute only to coherent tunneling.

8 Current Expressions

For coherent channels:

$$I_{\text{coh}} = \frac{2q}{h}\int T(E_z)\big[f_L(E) - f_R(E)\big]\,dE.$$

For inelastic channels (Meir–Wingreen):

$$I_{\text{SCBA}} = \frac{q}{h}\int \text{Tr}\Big[\Gamma_R G^{<} - \Sigma^{<}_R A\Big]\,dE.$$

The total current is the weighted sum over all transverse-energy slices.

9 Outputs

The simulator produces:

- I–V characteristics (current and current density),
- Transmission-like spectra vs. bias,
- Band profiles at 0 V and peak current,
- Differential conductance (dI/dV) and IETS (d^2I/dV^2),
- (New) Doping-dependent I–V sweeps stored in CSV.

10 Role of ATK and NEMO5 in This Workflow

The present simulator is a flexible, research-grade tool ideal for exploring:

- mode-selection mechanisms,
- SCBA behavior,
- defect-induced inelastic features,
- transverse-mode contributions,
- doping sweeps and Fermi-level shifts.

However, for larger-scale or more accurate modeling, two external tools fit naturally:

10.1 QuantumATK (Synopsys)

Best for:

- extracting material parameters from first principles (DFT),
- accurate band offsets, effective masses,
- phonon spectra and electron–phonon coupling,
- generating Wannier-based tight-binding Hamiltonians.

ATK serves as a high-accuracy *materials* engine whose outputs can be fed into this NEGF code.

10.2 NEMO5 (Purdue/Notre Dame)

Best for:

- large-scale atomistic NEGF (up to millions of atoms),
- full 3D Poisson–NEGF self-consistency,
- realistic scattering: phonons, impurities, alloy disorder,
- device-level validation of RTDs, TFETs, nanowires.

NEMO5 acts as a final *device-scale* verification tool for publication or experimental comparison.

11 Conclusion

This simulator provides a fast and flexible framework for studying coherent and inelastic resonant tunneling in GaAs/AlAs RTDs. With the new doping-dependent Fermi-level calculation and optional benchmarking against ATK and NEMO5, it forms a complete multi-scale workflow suitable for research on nanoscale tunneling, molecular sensing, and advanced quantum transport phenomena.