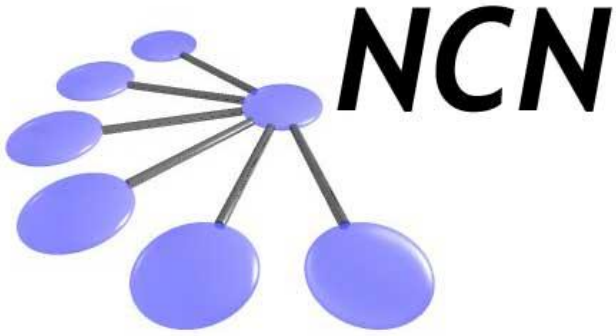
Resonant Tunneling Diode Simulation with NEGF (RTD NEGF) Tool Guide



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Simulation tool for studying electrical characteristics of GaAs/AlGaAs coherent RTDs

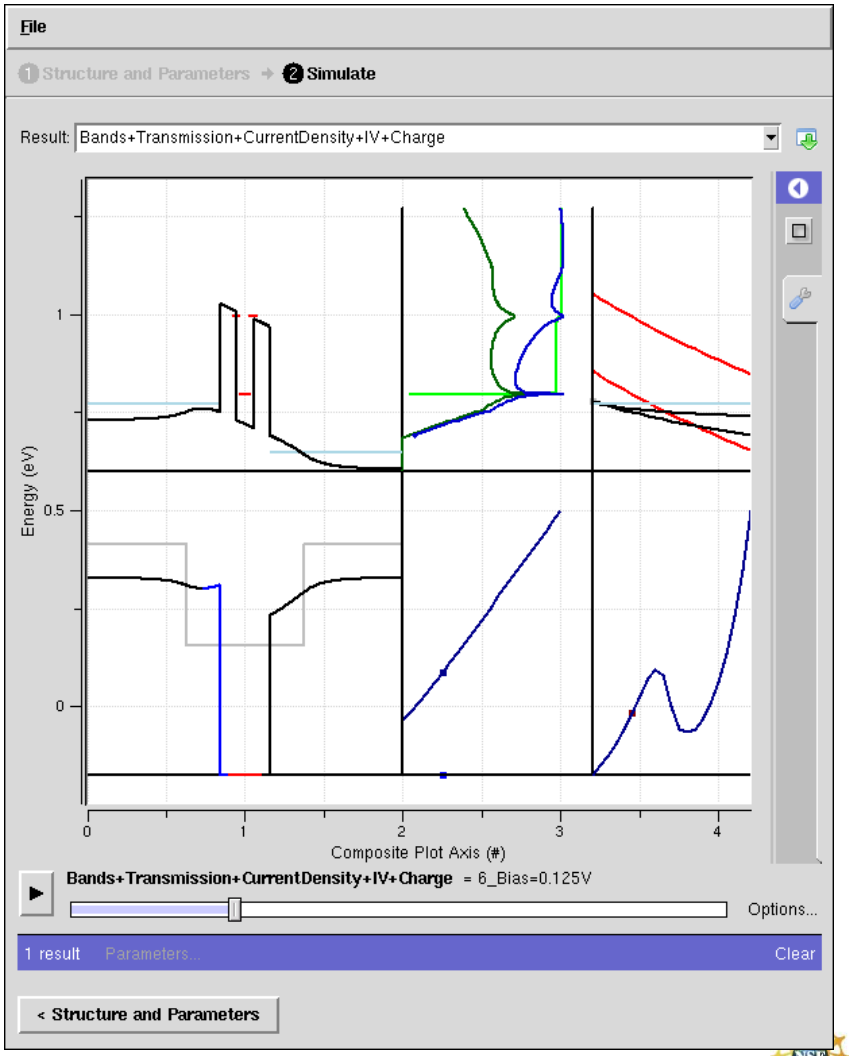
Features

- Two different options for computing electrostatic potential
  1. Thomas-Fermi method (Semiclassical)
  2. Hartree method (NEGF Quantum charge self-consistent)

- **Electron transport** using NEGF formalism with effective mass Hamiltonian

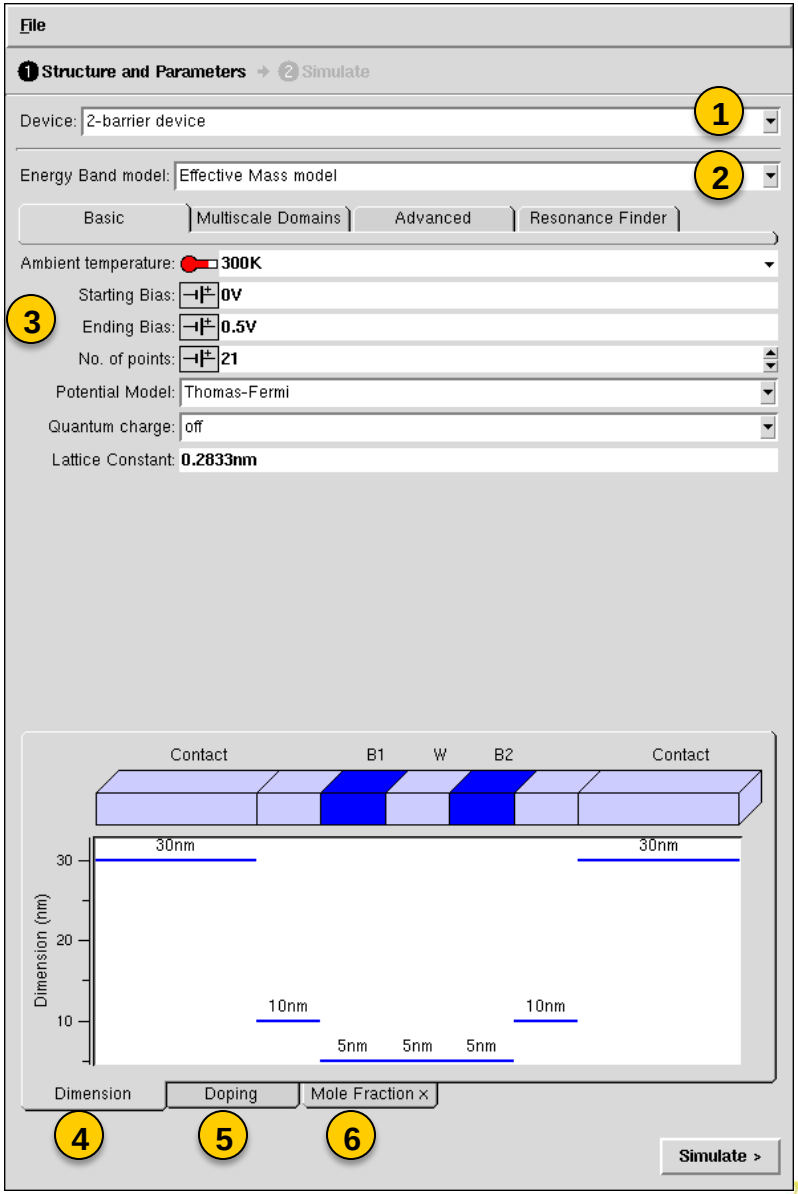
- Relaxation in emitter reservoir treated using an imaginary optical potential term (iη) in the self-energy calculation

- 2 barrier and multiple barrier RTDs



RTD NEGF - User Options

1. RTD type (number of barriers)
2. Band model for NEGF calculation
   - Effective mass (currently supported)
   - sp3s* (future release)
   - sp3d5s* (future release)
3. Input options classified into
   - Basic
   - Multiscale domains
   - Advanced
   - Resonance finder
4. Dimensions in nm
5. Doping in /cm3
6. Mole-fraction for AlGaAs



Basic Options

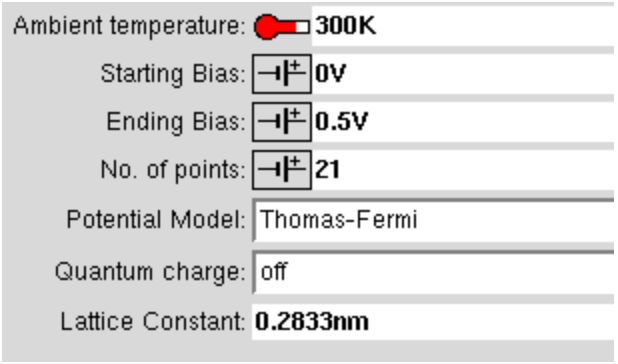
1. **Ambient Temperature** - Temperature value that will be used for the Fermi functions. Default options include 300K (room temperature) and 77K (liquid Nitrogen boiling point).

2. **Starting Bias** - Bias voltage at which the emitter terminal will be held fixed.

3. **Ending Bias** - The collector terminal voltage will be ramped up from the starting bias voltage value to this value.

4. **No. of Points** - Determines the bias voltage steps.

5. **Potential Model** - Thomas-Fermi or Hartree.



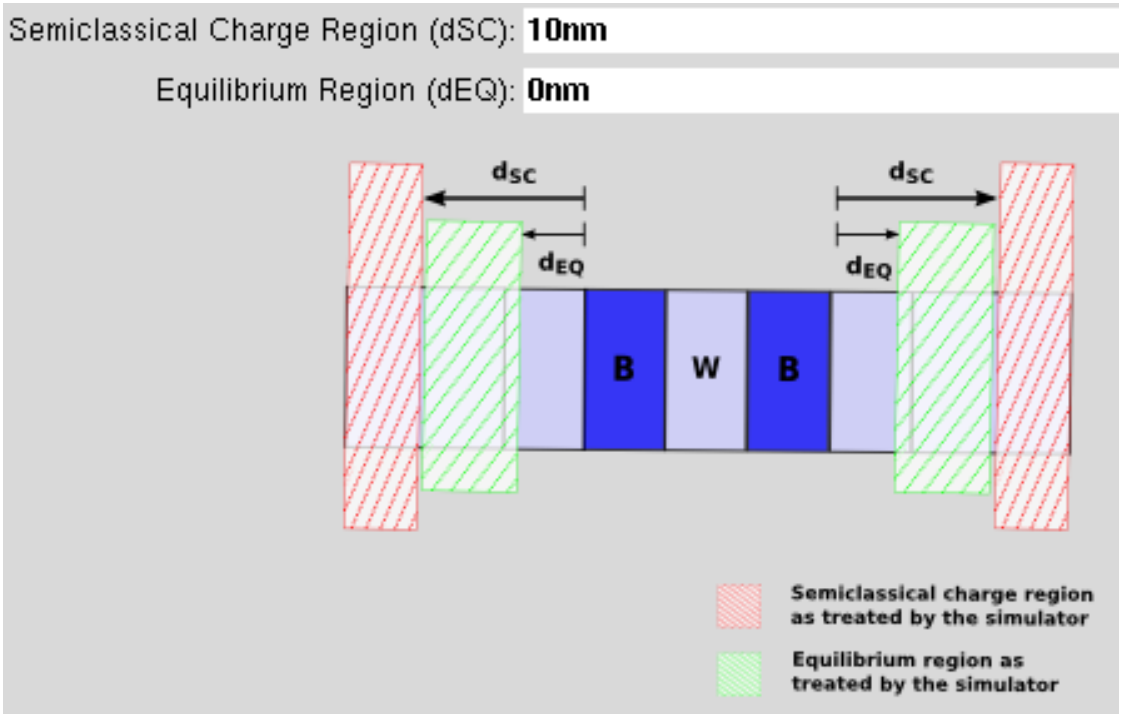
6. **Quantum Charge** - ON/OFF option that is enabled only for Thomas- Fermi simulation. If this option is set to be OFF then only semiclassical Thomas-Fermi charge will be displayed. If set to be ON then quantum charge resulting from NEGF transport calculation will also be displayed.

7. **Lattice Constant** - Determines real space grid size. Normally half the lattice constant of the unit cell. In other words thickness of one monolayer of the substrate.

Multiscale Domains Options

1. **Semiclassical charge region** - Region where charge is treated semiclassically. This is used for calculating charge for Hartree model and also for transport calculation for both Thomas-Fermi and Hartree models. Usually the region defined as terminal with flat band conditions and in equilibrium.

2. **Equilibrium region** – Region where the reservoir relaxation model is used.



Advanced Options

1. **Not-normalized Current Plot** - Switching this option to OFF will show the normalized current density plot.

2. **Resonances Scatter Plot** - The resonance vs voltage plot will appear as a scatter plot.

3. **Carrier Distribution Surface Plots** - Turning this option ON will display the energy resolved electron density profile.

4. **Reservoir Relaxation Model** - Option to choose the energy dependence of η used to account for scattering in the equilibrium reservoir. η can be made to reduce exponentially with energy below the emitter quasi-bound state or in a Lorentzian fashion or in a fixed manner.

5. **Reservoir Relaxation Energy** - For exponential and Lorentzian roll-off, this determines the maximum energy value of η.

6. **Decay Length** - For exponential and Lorentzian roll-off, this determines how fast with energy η reduces.

7. **Use Adaptive Energy Grid** - Can be used to control whether an adaptive energy grid or a fixed energy grid is used for calculation of NEGF charge, transmission and current.

8. **Poisson Criterion** - Convergence criterion used for Poisson equation.

Resonance Finder Options

1. **Resonance Finder** - Option to turn ON/OFF display of resonances and wavefunctions.

2. **No. of homogeneous grid points** – No. of energy grid points used by resonance finder
3. **No. of points per resonance**
4. **No. of points for Ec EF**
5. **Lanczos iteration step size** - Option for algorithm used to roughly estimate the location of resonances along energy axis.

6. **Lanczos iteration limit** - Option for algorithm used to roughly estimate the location of resonances along energy axis.

7. **Newton iteration step size** - Option for algorithm used to narrow down the energy location of the estimated resonance.

8. **Newton solver convergence condition** - Option for algorithm used to narrow down the energy location of the estimated resonance.

9. **Left exclusion region** - Region to the left of the 1st barrier that will be excluded from the spatial domain used for determining resonance wavefunctions.

10. **Right exclusion region** - Region to the right of the last barrier that will be excluded from the spatial domain used for determining resonance wavefunctions.

Outputs

1. Conduction band profile
2. Resonance energies & emitter quasi bound states
3. Wavefunctions for resonances & emitter quasi bound states
4. IV
5. Current density
6. Cumulative current density
7. Transmission
8. Electron density
9. Energy resolved electron density profile
10. Sheet density
11. Resonance vs voltage
12. Resonance width vs voltage