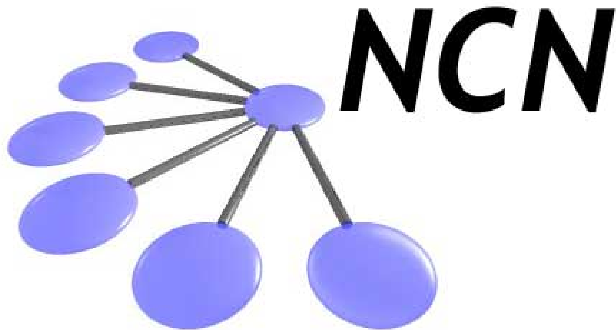


Nanowire2.0

First time user's guide

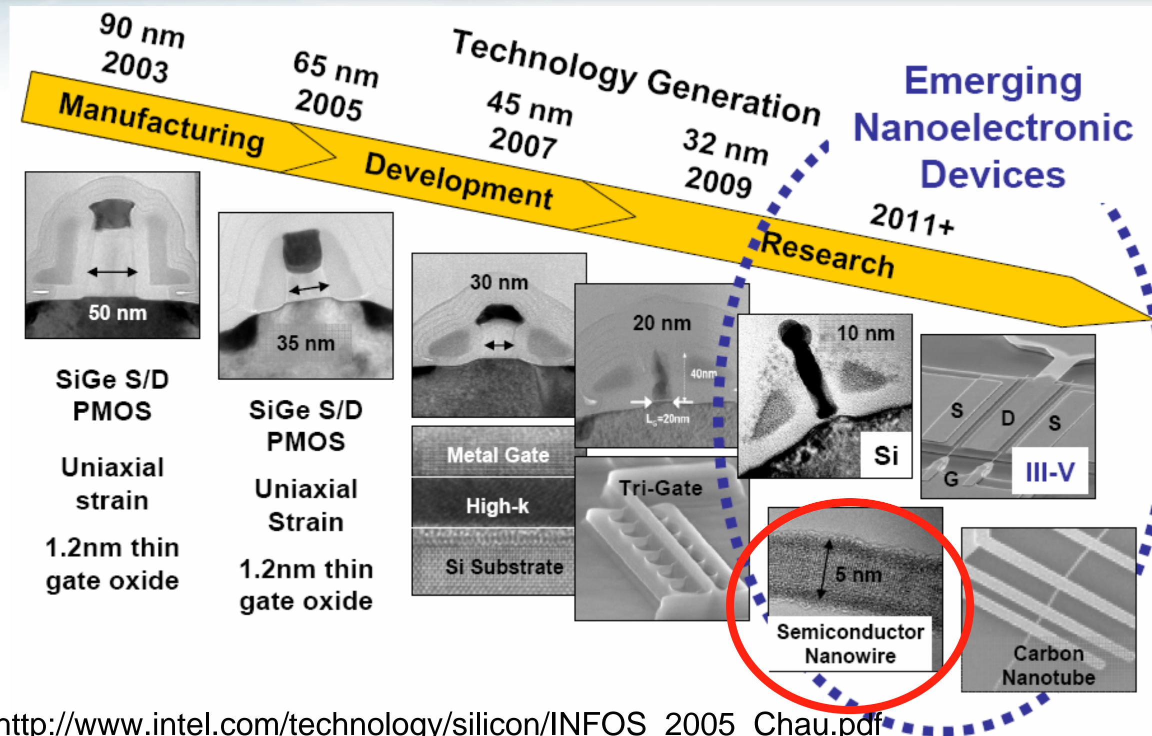
April, 2008

Saumitra R Mehrotra

Overview

- **Why the need for simulator.**
- **Rappture Input parameters.**
- **Transport Models used.**
- **Rappture Output.**
- **Examples**
- **References**

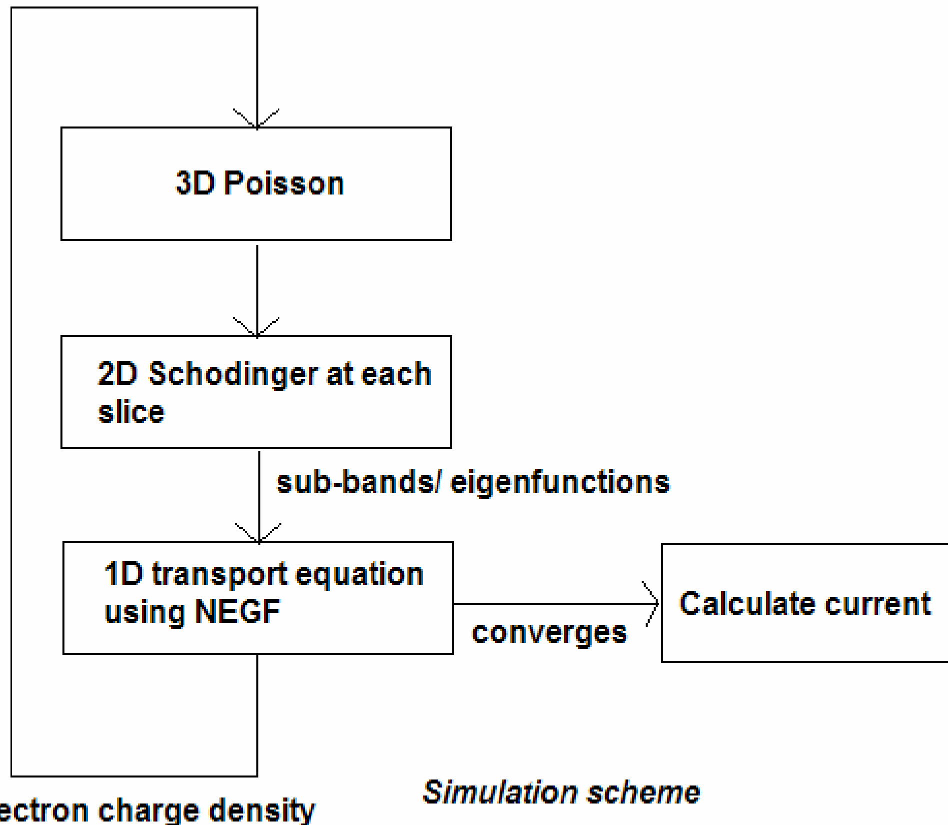
Why the need for simulator?



[1] http://www.intel.com/technology/silicon/INFOS_2005_Chau.pdf

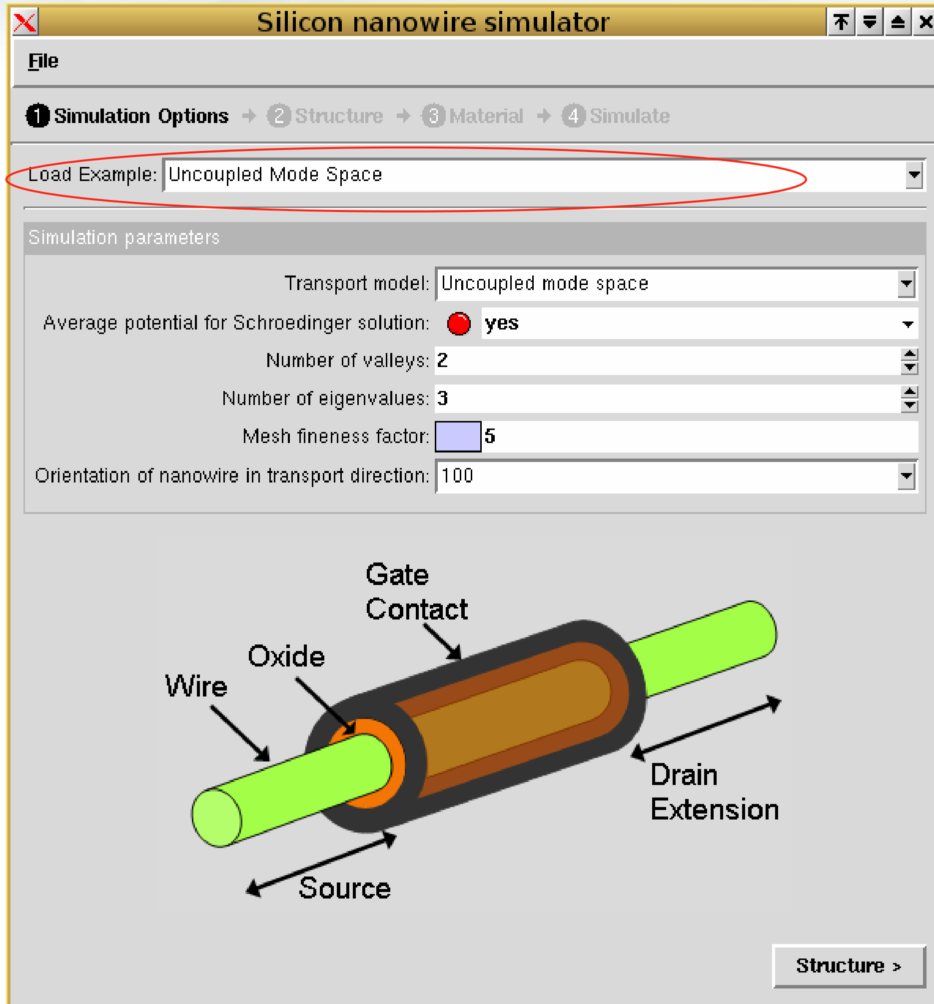
- Nanowire devices are emerging future nanoelectronic devices.
- Need to look beyond Drift-Diffusion modeling approach as channel lengths approach ~ 10nm and transport is nearly ballistic.

Why the need for this simulator?



- 'Nanowire' is full Non-Equilibrium Green's Function (NEGF) based 3D simulator [2],[3].
- Performs quantum simulation based on effective mass approach.
- Self-consistent solution of 3D Poisson with 1-D transport equation.
- Option of ballistic and scattering regimes.

Rappture Input: Simulation Options

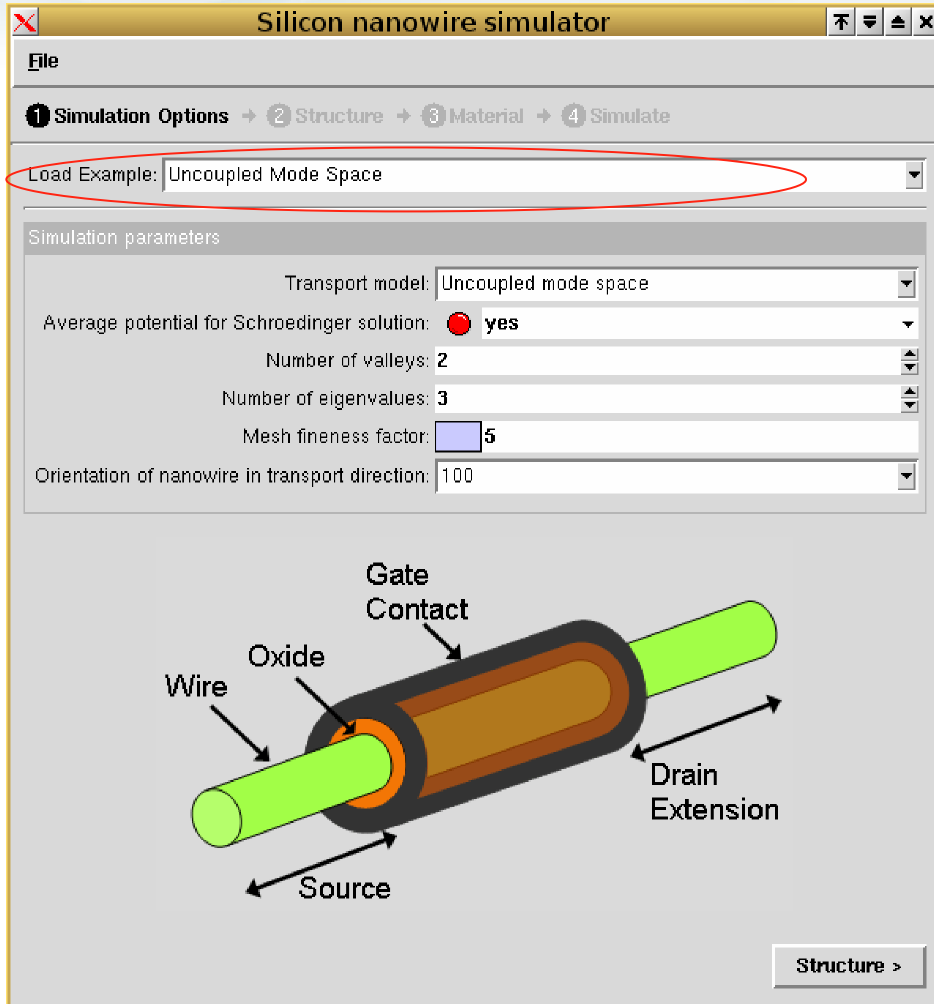


Load Example

- The Rappture input Interface provides 4 examples which can be loaded without running a simulation.

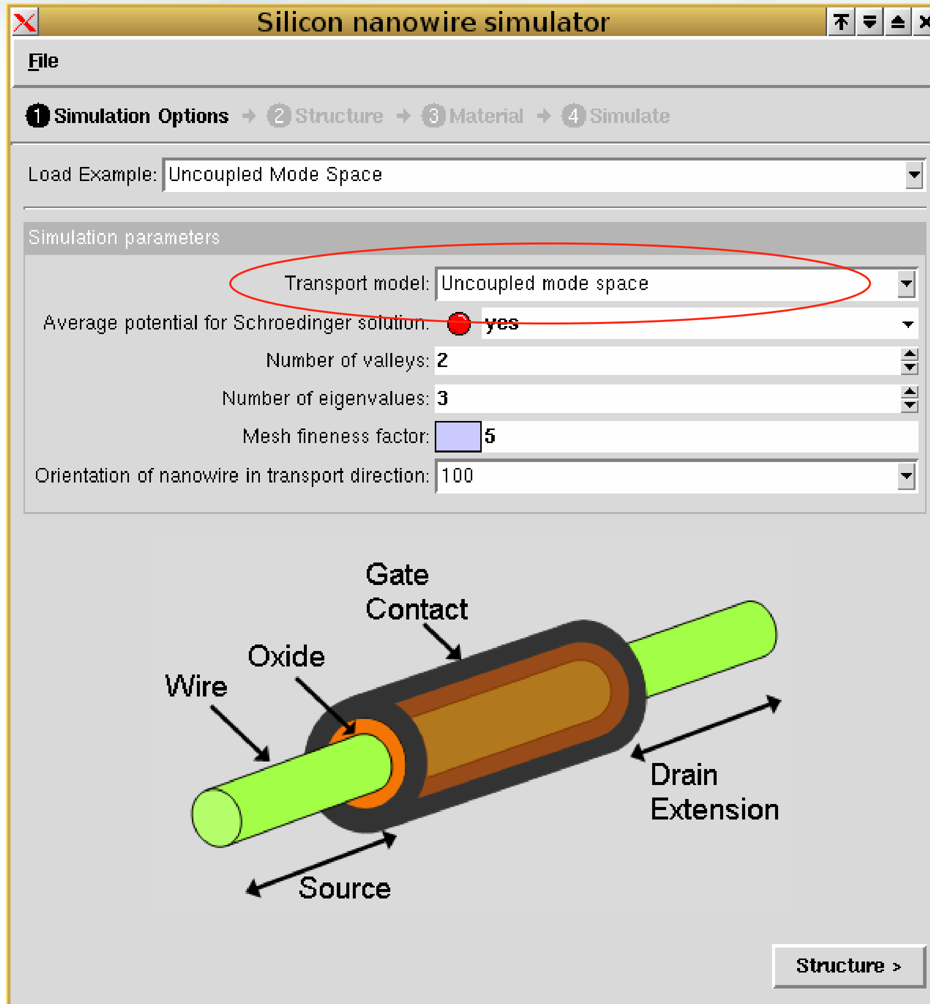
- (1) *Channel formation* – In this example one can view the channel formation at low drain and high gate bias.
- Electrons are pulled into the channel as gate voltage is increased.

Rappture Input: Simulation Options



- (2) *Uncoupled Mode Space (UMS)* – This is a default run for UMS with averaging option turned ON.
- (3) *Coupled Mode Space (CMS)* – This is a default run for CMS with averaging option turned ON.
- (4) Uncoupled Mode Space with Scattering – This is the default run in scattering mode with scattering option turned ON.

Rappture Input: Simulation Options



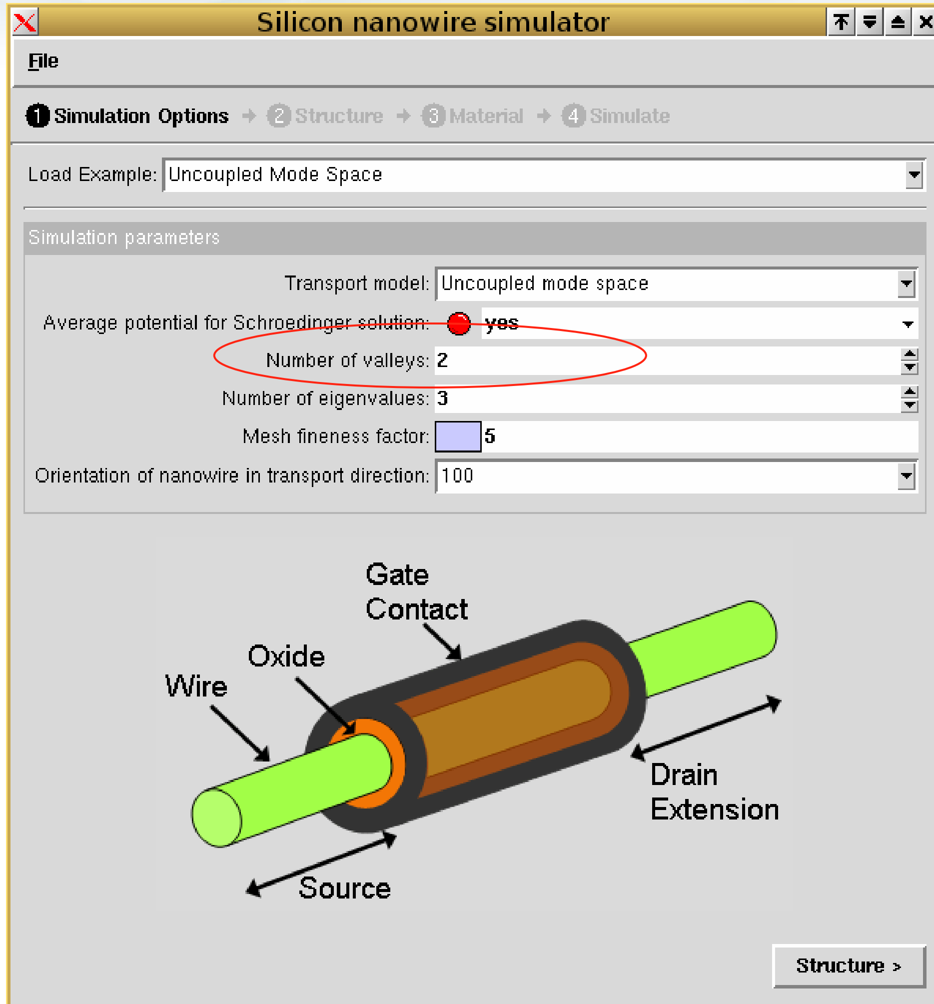
Transport model

- Rappture input provides with three options for the Transport model.
  - » UMS
  - » CMS
  - » UMS with scattering

Transport models have been explained in a later section.

Also refer [2],[3] for the mathematical treatment used.

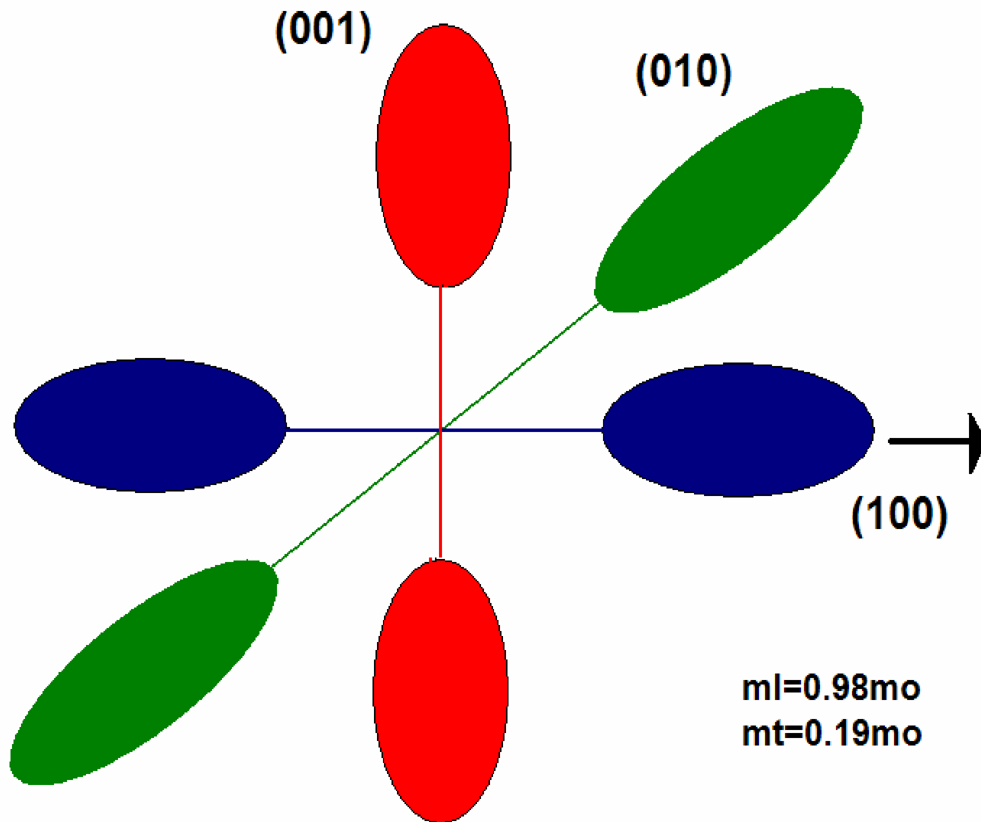
Rappture Input: Simulation Options



Number of valleys

- Here the user can select the number of valley pairs (1-3) to be included in the transport model.
- Silicon has six valleys as shown in the figure in next slide.
- For (100) orientation selecting Number of valleys=2 will be a good option.
- For (111) and (110) Number of valleys=3 is recommended.

Rappture Input: Simulation Options



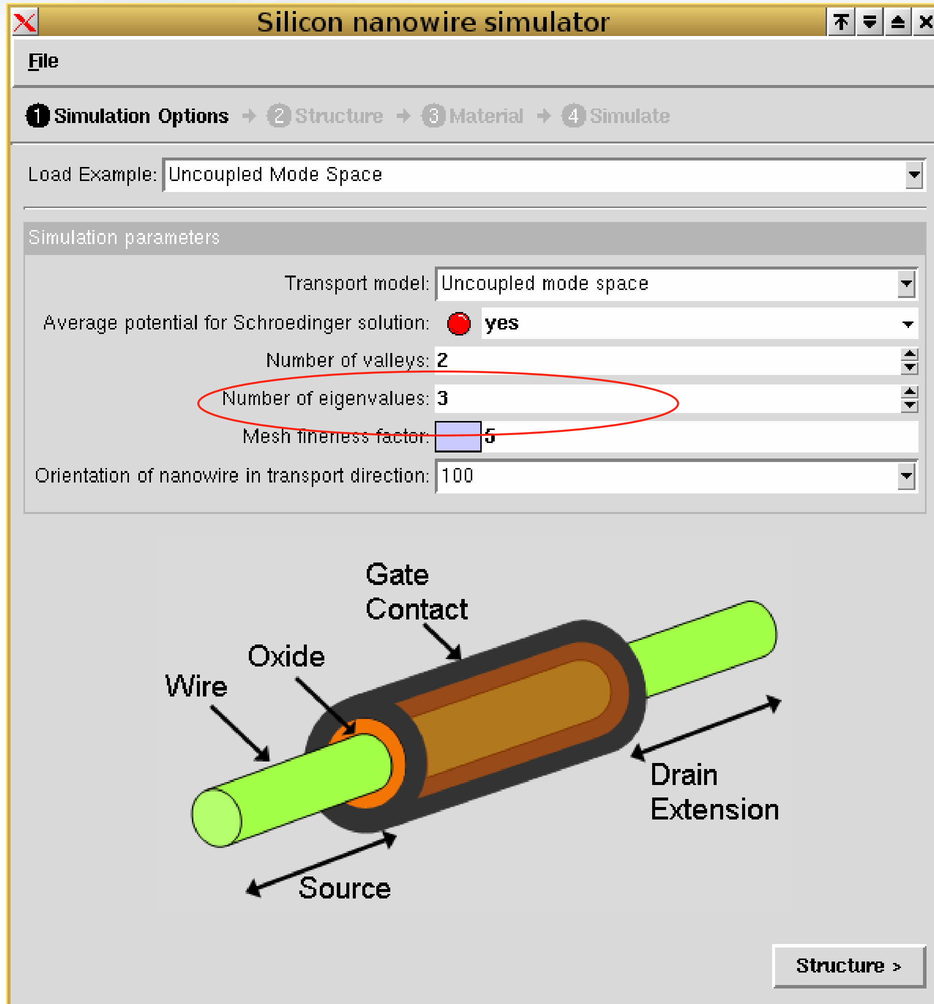
Number of valleys

Silicon in (100) transport direction has 4 valleys (2 pairs) parallel to transport direction while 2 valleys (1 pair) perpendicular to the transport direction.

- number of valleys=1 includes the (001) pair (red).
- number of valleys=2 includes the (001) and (100) pair (red and blue).
- number of valleys=3 includes all the pairs.

nanoHUB online simulation and more — an NCN project

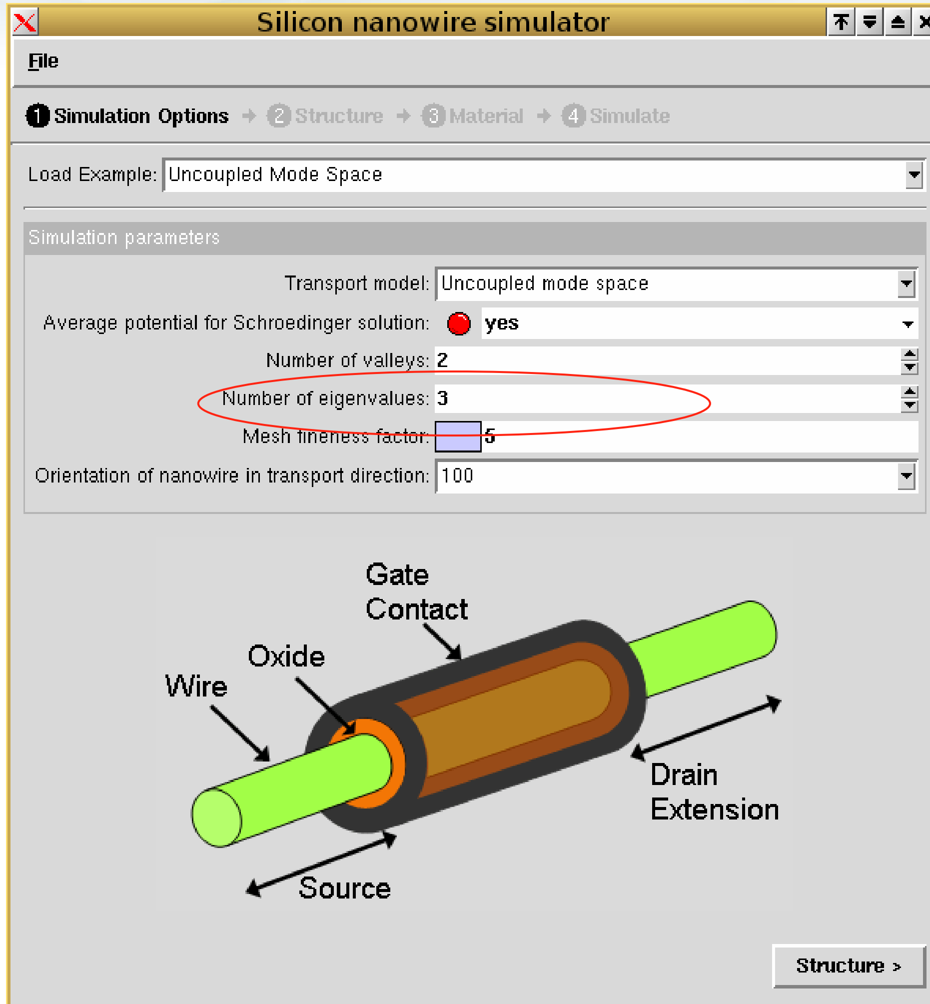
Rappture Input: Simulation Options



Number of eigenvalues

- It is the number of modes available for electron transport.
- More the number of modes more channels are available for transmission (conductance).
- Number of modes available increases with increasing diameter of the wire.
- Since here we simulate only a few number of modes it should be selected commensurately with the diameter.

Rappture Input: Simulation Options

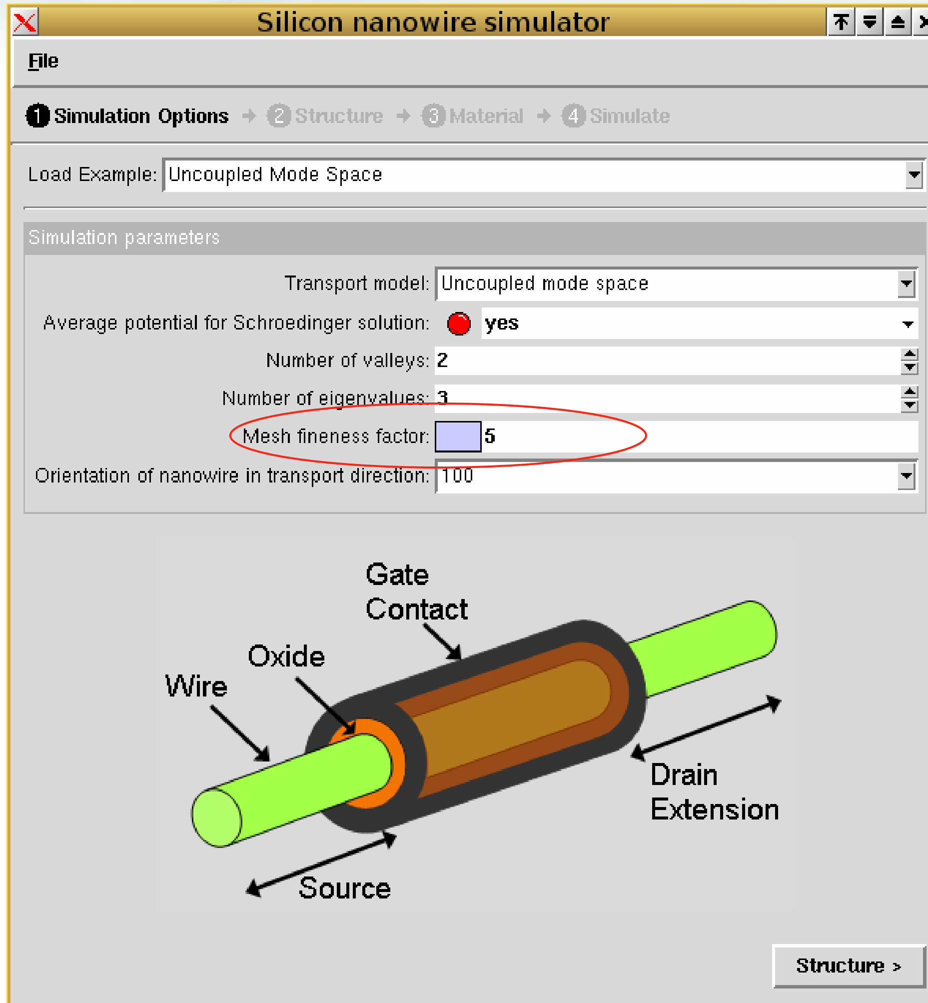


Number of eigenvalues

- As a thumb rule one can refer to the following table to capture >99% of current.

Diameter	Number of modes
3 nm	1
6 nm	3
12 nm	13

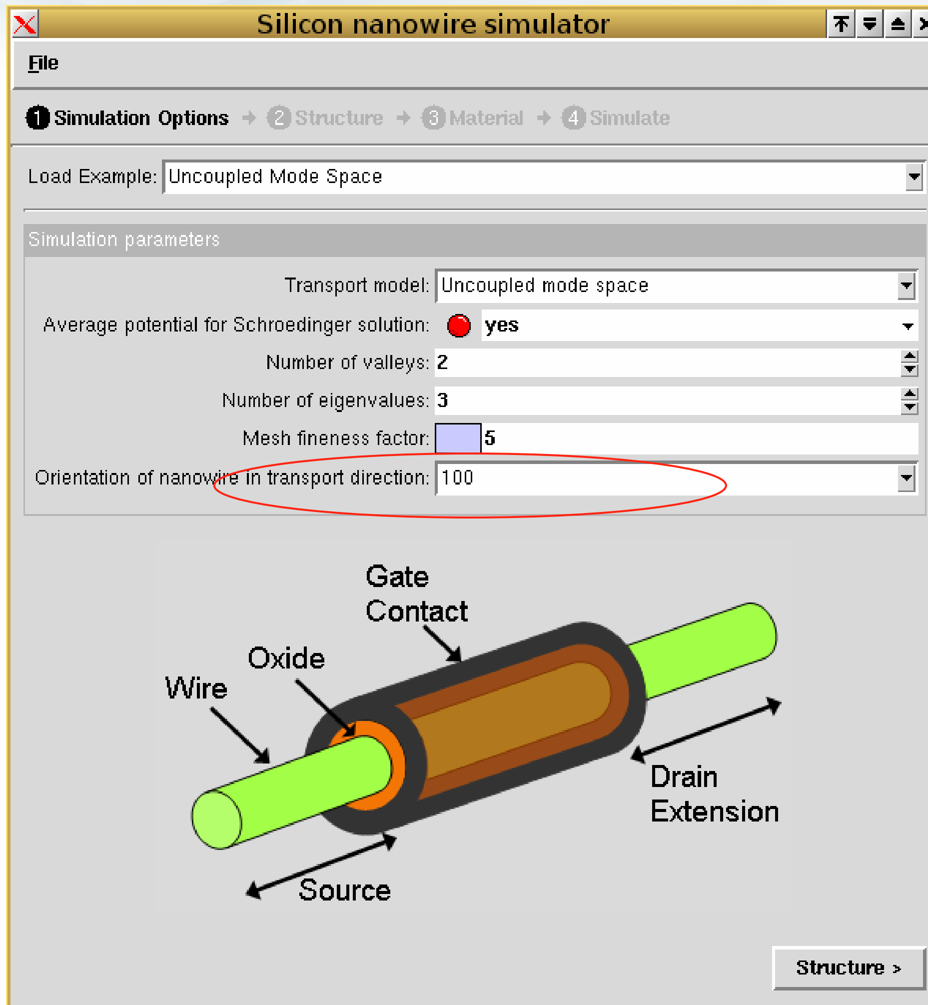
Rappture Input: Simulation Options



Mesh fineness factor

- Mesh fineness factor determines the fineness of the triangulated 2D mesh.
- User can vary the factor from 1-20, with 1 being most coarse and 20 being most fine.
- Increasing the fineness factor will also increase the simulation time.

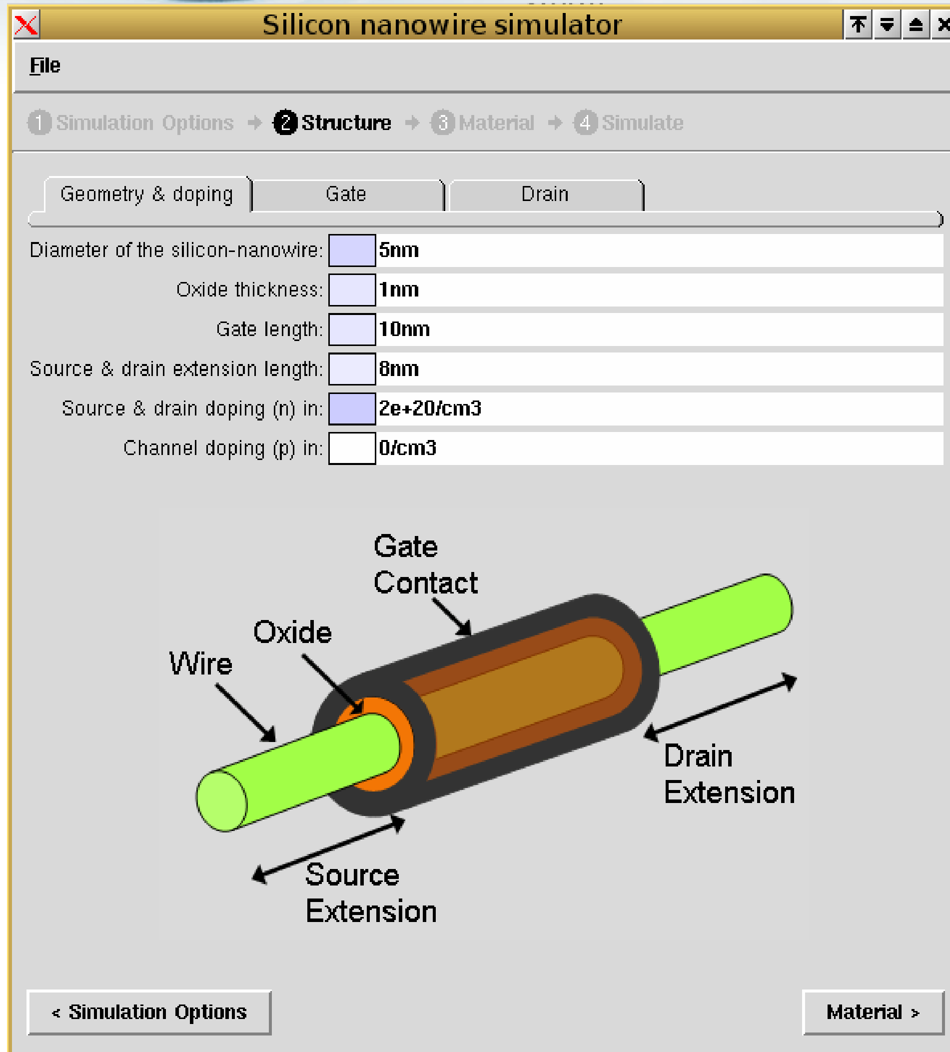
Rappture Input: Simulation Options



Orientation of nanowire in transport direction

- User can choose from three different transport orientations i.e. (100) , (110) and (111).
- The orientation inbuilt is only at first order with masses along different directions calculated from [4].

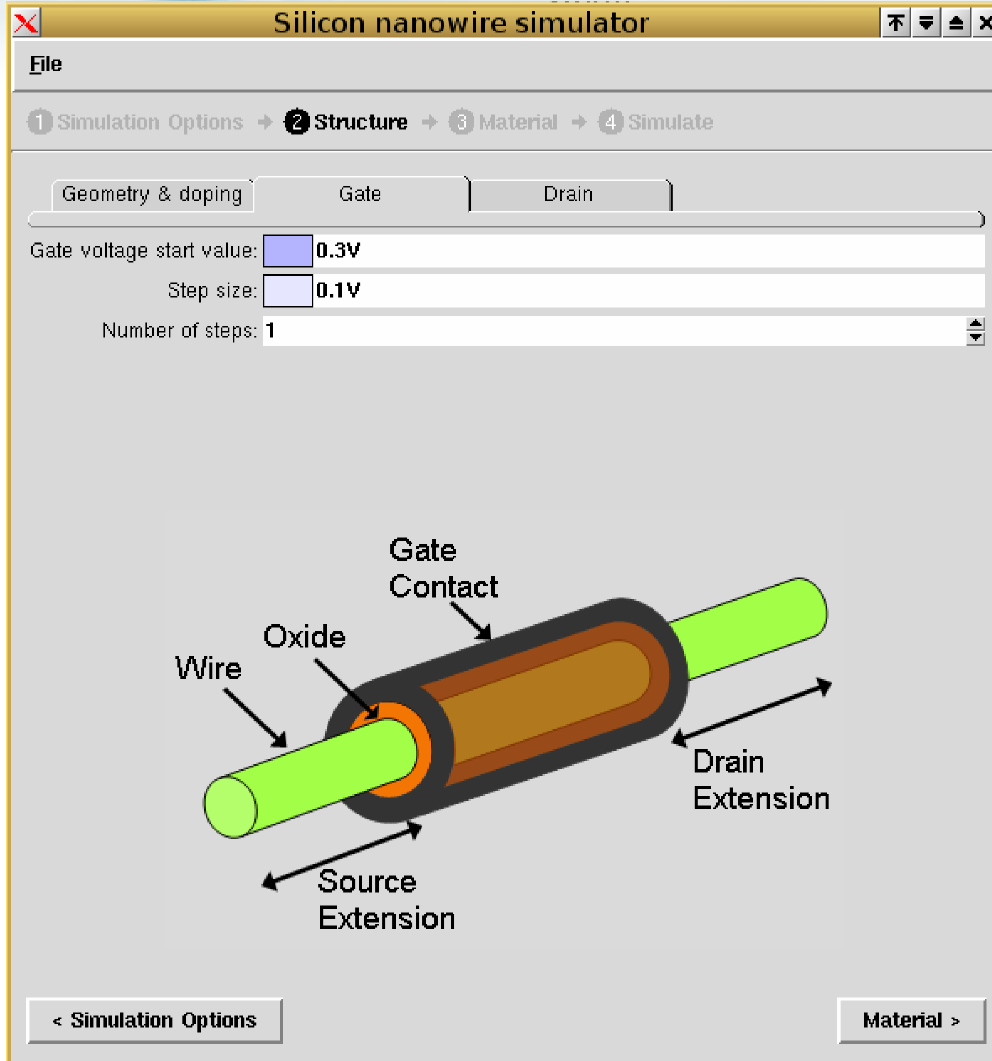
Rappture Input : Structure



Geometry & Doping

- Diameter of the silicon nanowire – Defines the diameter in nanometers (nm) for silicon nanowire.
- Oxide thickness – Defines the oxide thickness around the circular nanowire in nm.
- Gate length – Defines the gate length for the nanowire in nm.
- Source & drain doping (n) – Defines the n-type doping level for source and drain regions
- Channel doping (p)-Defines the p-type channel doping. Abrupt doping profiles have been used in this simulator

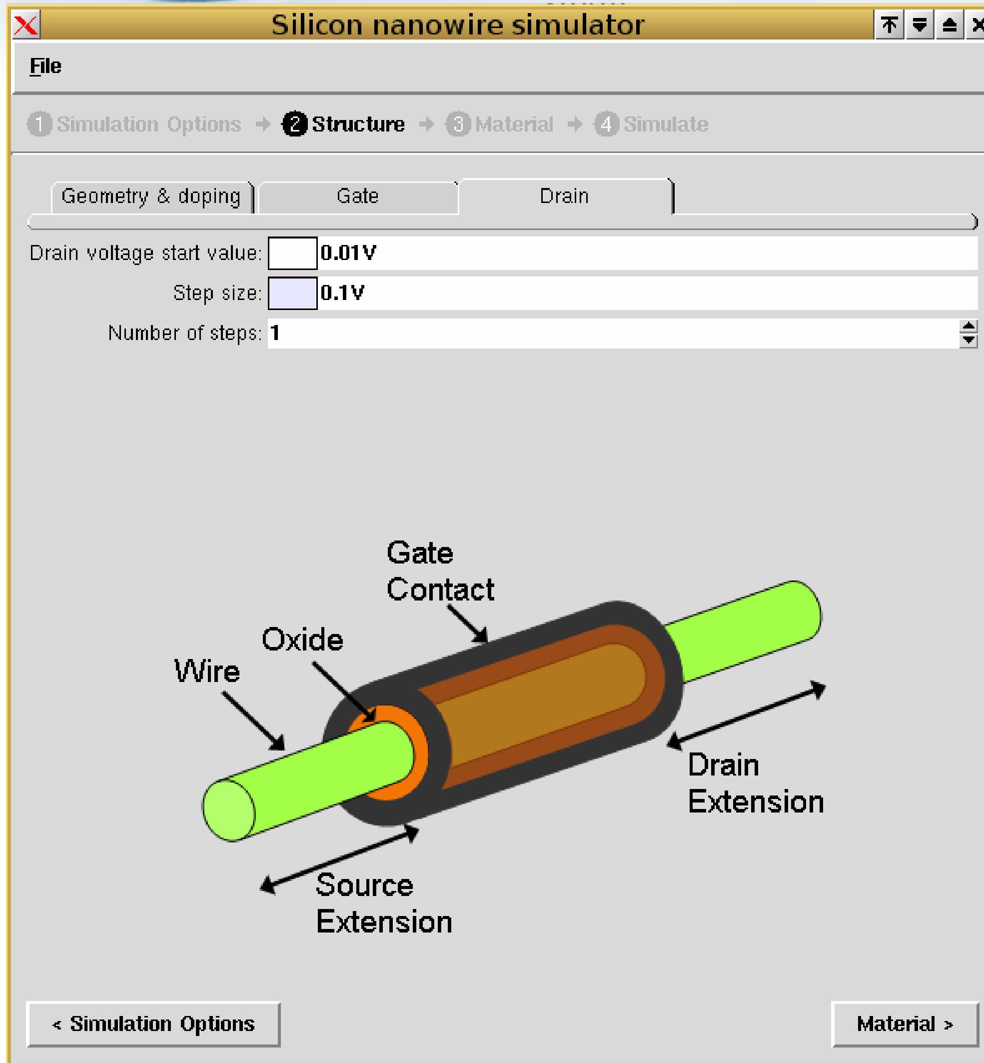
Rappture Input: Structure



Gate

- Here the user can define
- Gate voltage start value (V)
- Step size (V), and
- Number of steps.

Rappture Input: Structure



Drain

- Here the user can define
- Drain voltage start value (V)
- Step size (V), and
- Number of steps.

Rappture Input : Material Properties

Silicon nanowire simulator

File

1 Simulation Options → 2 Structure → 3 Material → 4 Simulate

Material Properties

Gate work function:	4.05eV
Silicon Dielectric Constant:	11.9
Oxide Dielectric Constant:	3.9
Silicon work function:	4.05eV
Oxide work function:	3.1eV
Longitudinal Effective mass in silicon (Mo):	0.98
Transverse Effective mass in silicon (Mo):	0.19
Effective mass in dielectric (Mo):	0.4

Gate Contact

Oxide

Wire

Drain Extension

Source

< Structure

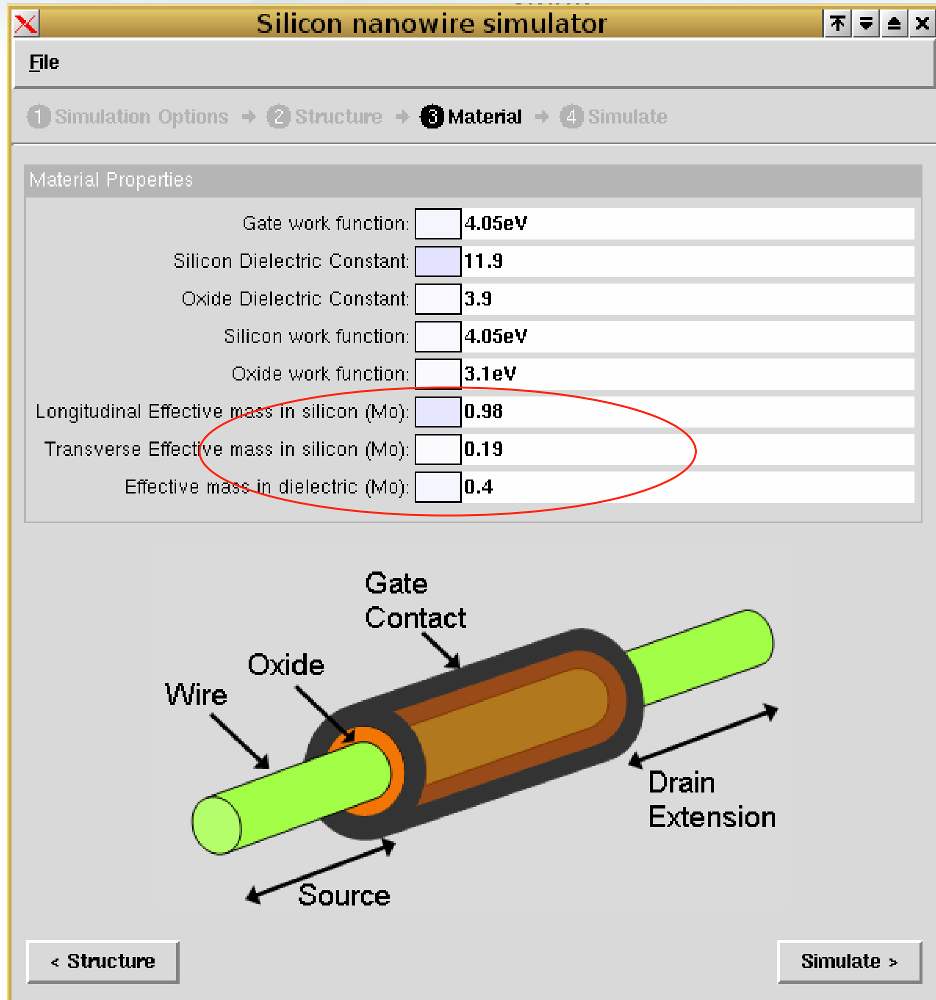
Simulate >

Material

Choose the material properties for the channel, insulator and gate material.

- Gate work function – Enter workfunction for gate material in eV.
- Silicon work function – Enter workfunction for Silicon (channel) eV.
- Silicon work function – Enter workfunction for Silicon (channel) eV.
- Silicon dielectric constant.
- Oxide dielectric constant.

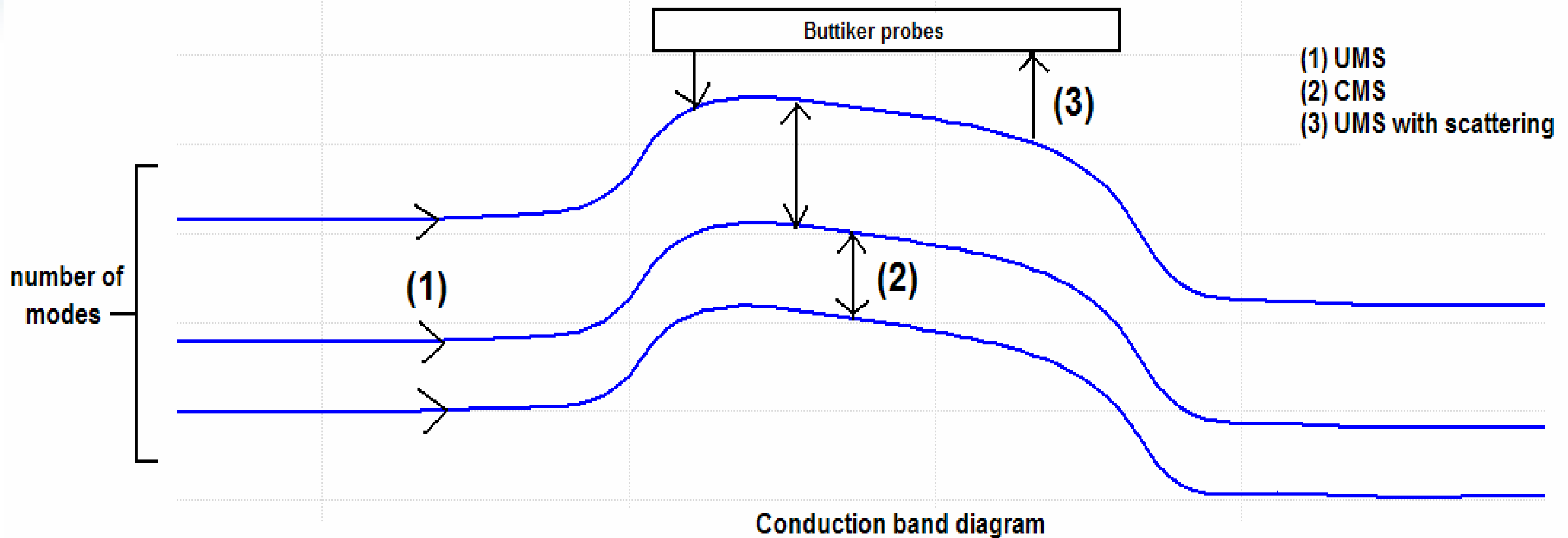
Rappture Input : Material Properties



Material

- Longitudinal effective mass – Defines the m_l for the silicon ellipsoid in terms of electron effective mass (m_o).
- Transverse effective mass – Defines the m_t for the silicon ellipsoid in terms of electron effective mass (m_o).
- Effective mass in dielectric – Defines the anisotropic electron effective mass in the diectric (oxide).

Transport Models



- A nanowire can be simulated with different number of modes given by 'Eigenvalues' option.
- Thicker diameter would require more number of modes while thinner wires can be simulated faithfully with fewer number of modes.
- Difference transport models used have been described in the next slide.

Transport Models

(1) Uncoupled Mode Space (UMS)

In uncoupled mode space the different modes for traveling electrons are decoupled. If an electron enters one mode it travels along that mode till the end. It can be treated as *n* 1D transport problem with *n* being the number of modes. (UMS is an approximation which works well as long as shape of the wire doesn't change along the length or there is on surface scattering)

(2) Coupled Mode Space (CMS)

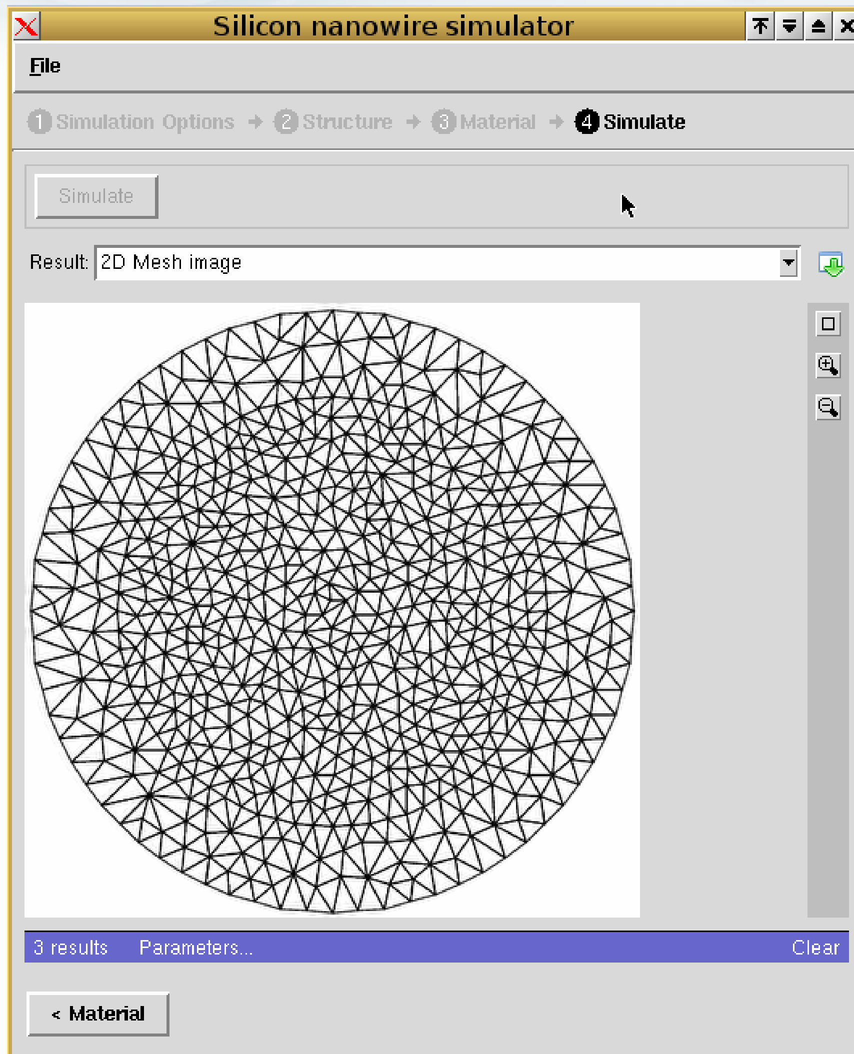
In coupled mode space the modes talk to each other i.e allows for mixing of electron modes. A CMS simulation would normally take much longer time as compared to UMS.

(3) Uncoupled Mode Space with Scattering

Scattering is introduced using the Buttiker Probe method. In this scattering method electrons are injected (generation process) and removed (recombination process) at random sites such that net electron exchange with the system is zero.

Refer [2] for further reference

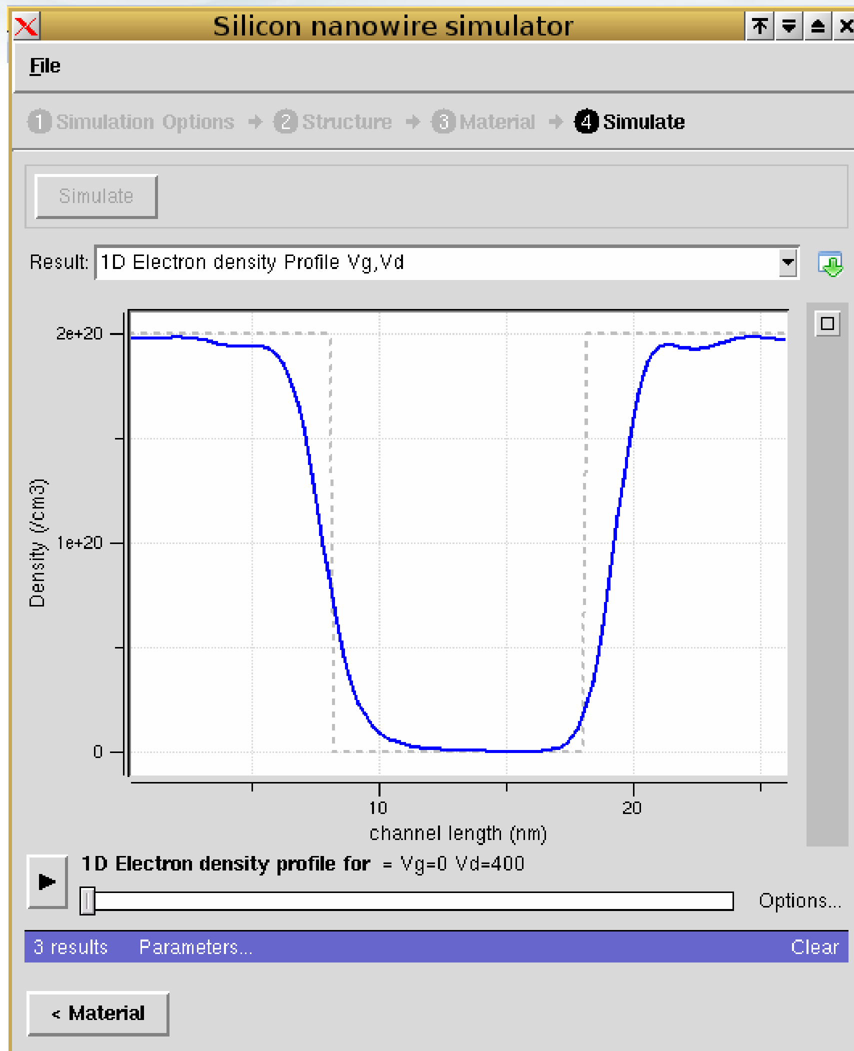
Rappture Output



2D Mesh Image

- The 2D mesh used for simulation for the nanowire is displayed in the output.
- The 3D mesh is created by spacing the 2D mesh at 0.2nm.
- Oxide region is about half as fine as the silicon region.

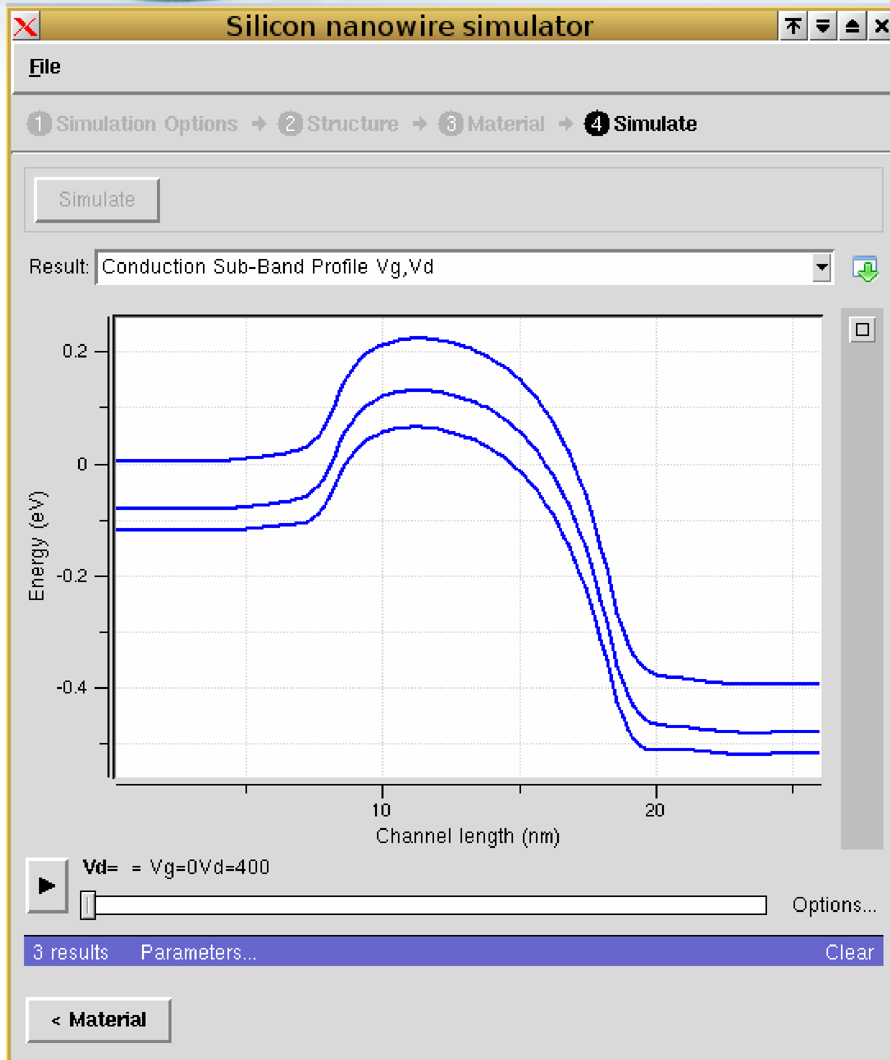
Rappture Output



1D Electron density

- Electron density along the channel for the nanowire is plotted in sequence with the Drain/Gate voltages.
- Initial doping profile for the nanowire can be seen in the background with dashed lines.

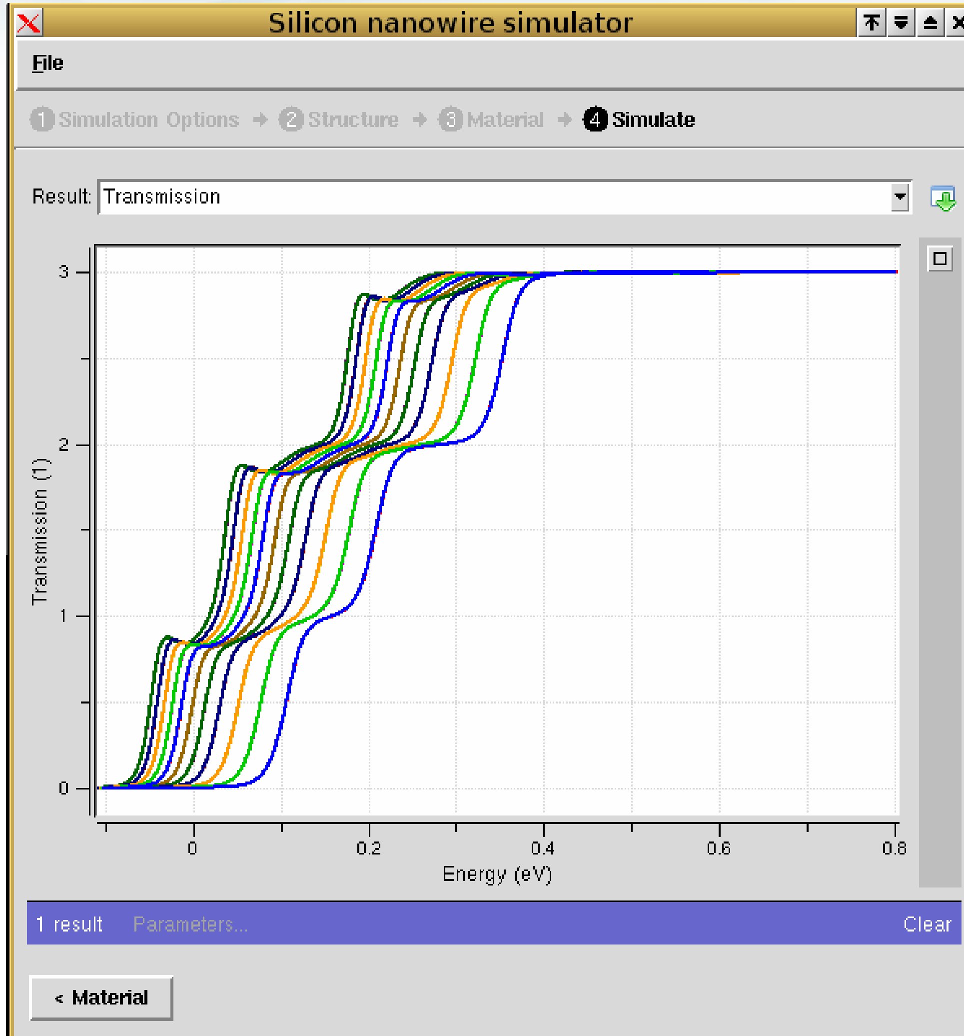
Rappture Output: Conduction sub-band Profile



Conduction sub-band profile

- Conduction sub-band profile for the device is plotted in sequence of gate/drain voltage.
- For UMS % current carried by each sub-band is specified as the modes work independently of each other (unlike for CMS case where there is mixing of modes).

Rappture Output



Transmission

- Transmission curves ,T(E) with energy are displayed in output.
- The steps in the figure here refer to each sub-band being included in the simulation at that energy level.
- The separation between the steps refer to difference in sub-band energies.
- The small peaks refers to *tunneling* of electrons beneath the barrier.

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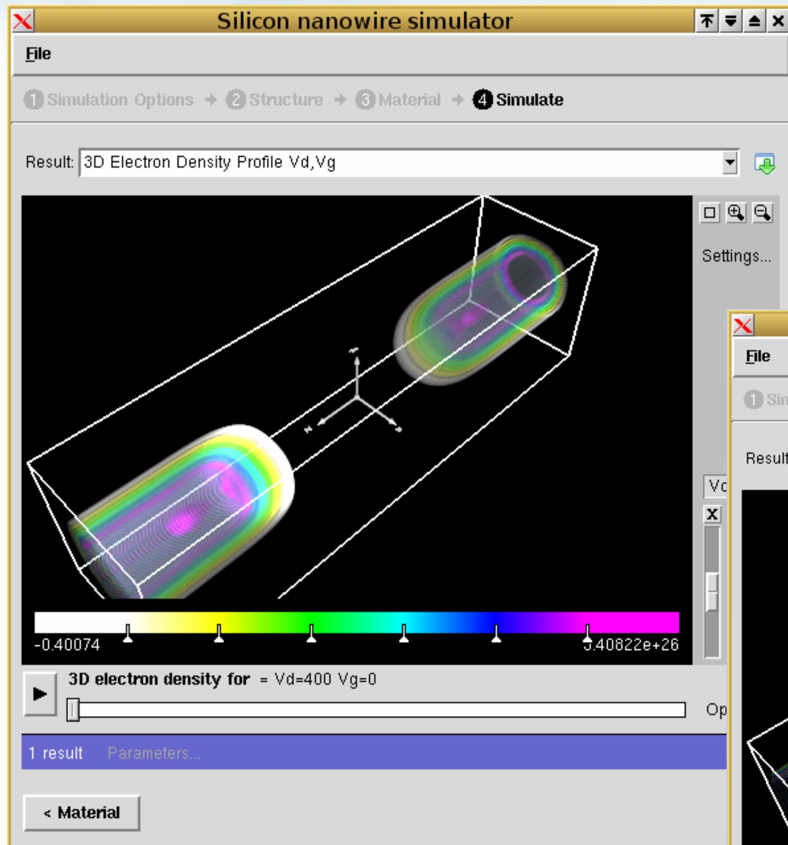
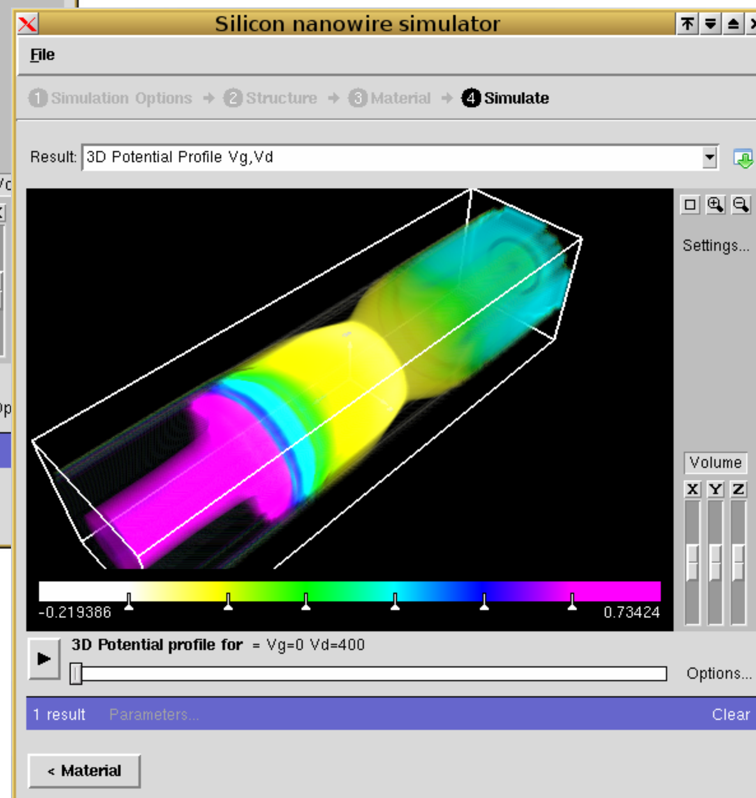
Rappture Output



3D electron density & 3D potential profile

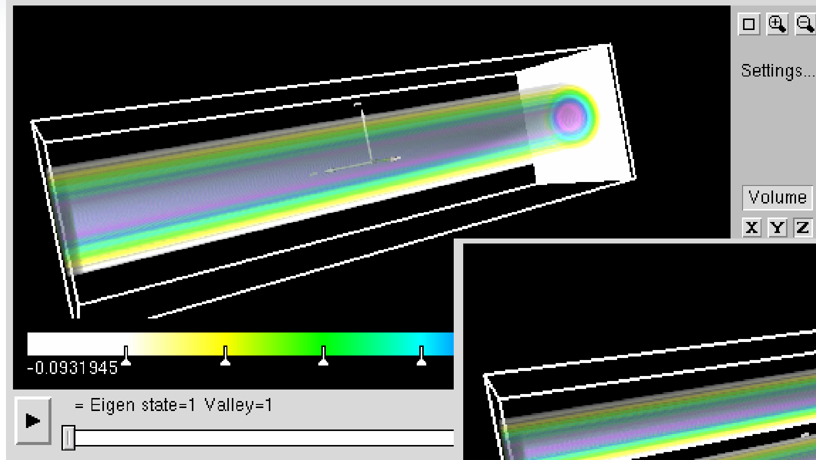
- User can view the 3D profiles at each applied bias in a sequence.

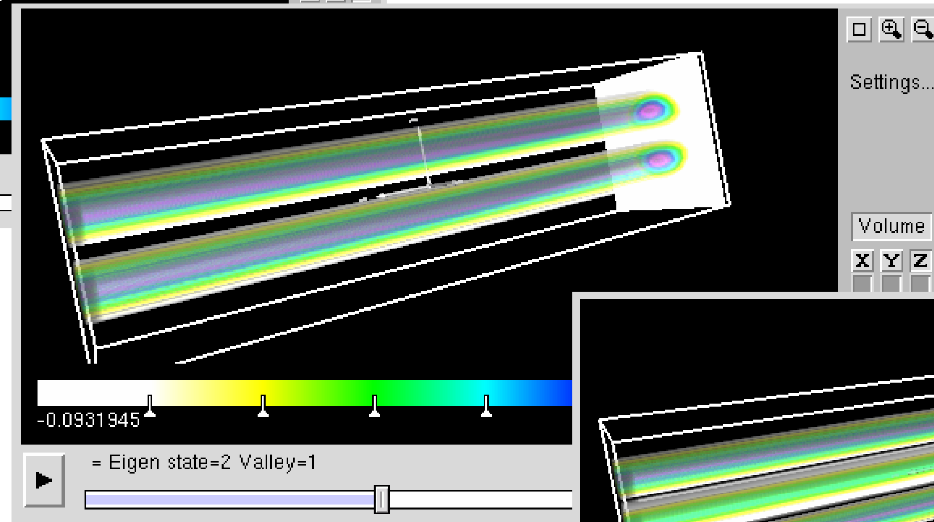


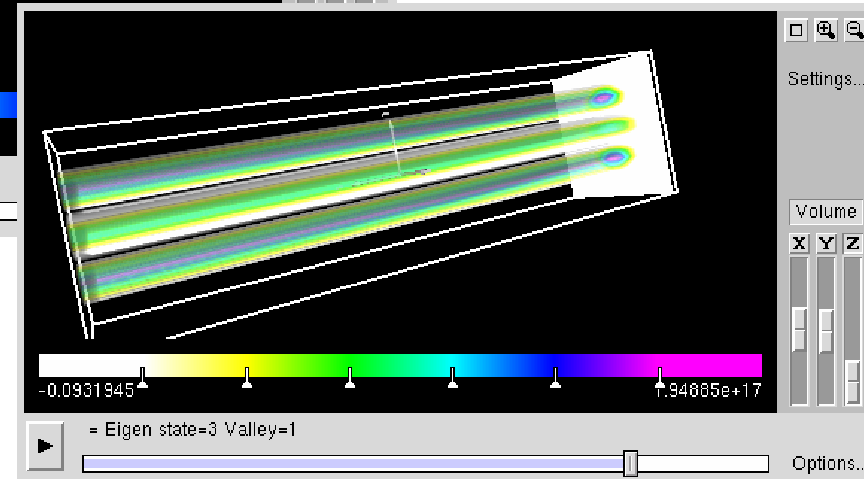
Rappture Output

3D Modes

- 3D modes for each eigen state (and valley) are displayed for initial and final bias points

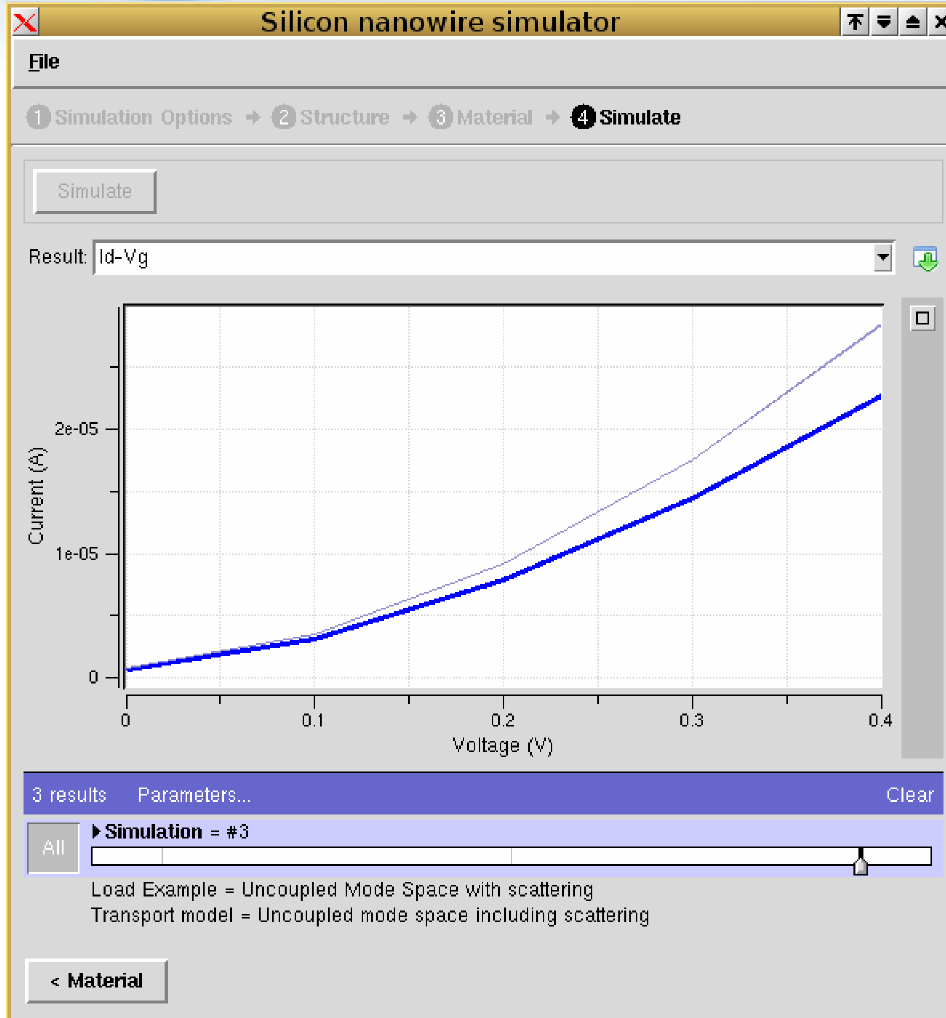






First three modes for (001) valley pair.

Examples



Comparison of Id-Vg for UMS/CMS/UMS with scattering for D=5nm and Lg=10nm.

- Here we can see that scattering leads to smaller output current.
- UMS and CMS models have very similar current values which validates the approximation used for UMS.

References

[1] http://www.intel.com/technology/silicon/INFOS_2005_Chau.pdf

[2] Jing Wang, Eric Polizzi, Mark Lundstrom, "A three-dimensional quantum simulation of silicon nanowire transistors with the effective-mass approximation," *Journal of Applied Physics* **96**(4), pages 2192-2203, 2004.

[3] Wang, Jing. Ph.D., Purdue University, August, 2005. Device Physics and Simulation of Silicon Nanowire Transistors. Major Professor: Mark S. Lundstrom.

[4] F Stern & W E. Howard, “Properties of semiconductor surface inversion layers in the electric quantum limit,” *Phys. Rev.* 163, pages 8l6-35,1967.

If you are using Nanowire results in a paper, please site [2]

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