



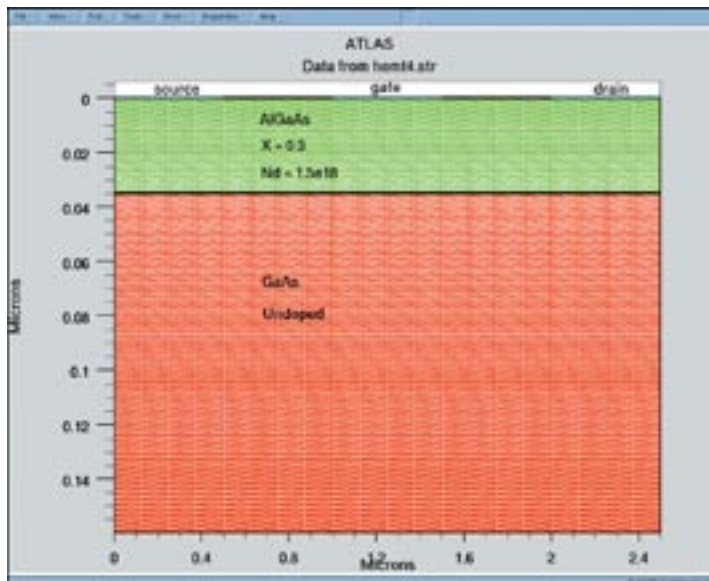
Quantum2D/3D

Simulation Models for Quantum Confinement Effects

Quantum provides a set of powerful models for simulation of various effects of quantum confinement of carriers in semiconductor devices. A self-consistent Schrodinger - Poisson solver allows calculation of bound state energies and associated carrier wave function self consistently with electrostatic potential in semiconductor devices. A Quantum moment transport models allow simulation of confinement effects on carrier transport. The Van Dort and Hansch models provide semi-empirical simulation of confinement effects on MOS devices. A multiple quantum well (MQW) provides specific models for gain and spontaneous recombination in light emitting devices.

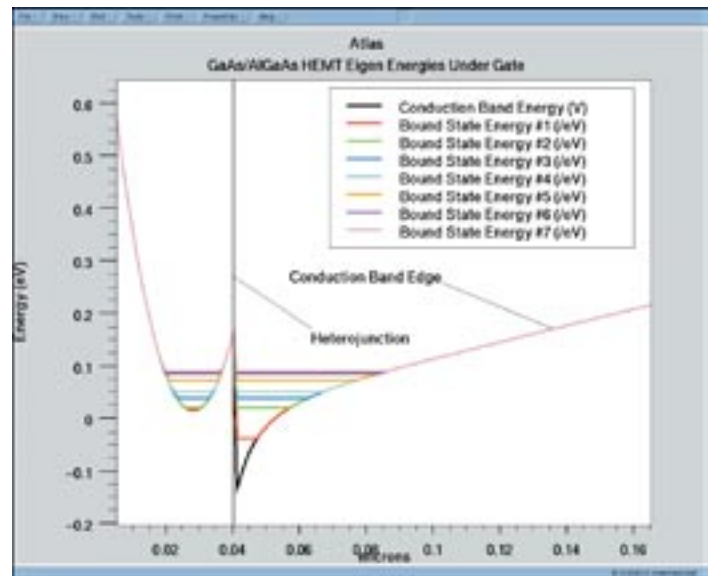
Schrodinger-Poisson

To model the effects of quantum confinement, Quantum allows the self-consistent solution of the Schrodinger equation with Poisson's equation. Poisson's equation is solved in two dimensions over the entire device while Schrodinger's equation is solved in one dimensional slices across the device. These solutions provide calculations of the bound state energies (Eigen energies), the carrier wave functions (Eigen functions), and carrier concentrations in the presence of quantum mechanical confining potential variations. This model can be used to estimate the charge control behavior of a device. Currently the Schrodinger-Poisson calculations are not coupled into the current transport equations and therefore this method will show no quantum effects in the current-voltage characteristics.

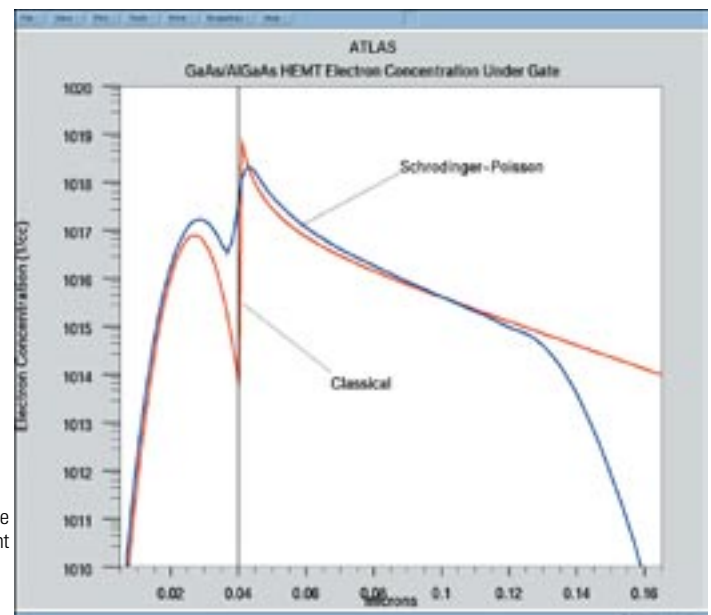


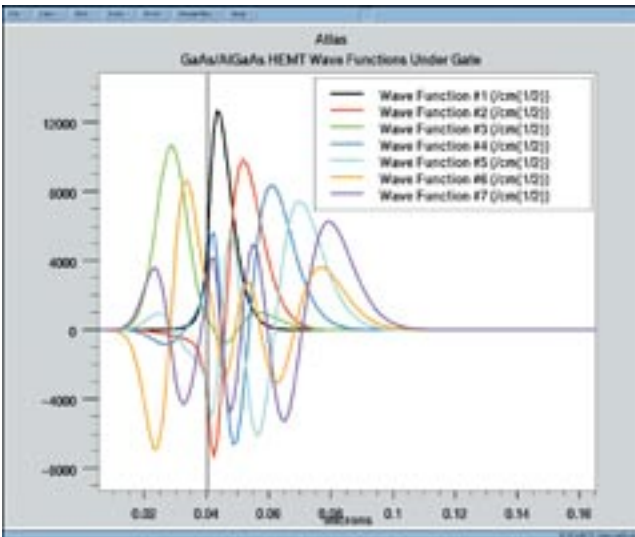
This is an example GaAs/AlGaAs HEMT device structure used for demonstration of the self-consistent solution of Schrodinger's equation and the Poisson equation. The device has an undoped GaAs substrate topped by a 0.35 micron layer of AlGaAs doped at $1.5 \times 10^{18} \text{ cm}^{-3}$, with a composition fraction of 0.3. It has a 0.5 micron gate.

This figure gives a comparison between the electron concentrations under the gate of the GaAs/AlGaAs HEMT device as predicted by the self-consistent Schrodinger-Poisson solution and as predicted by classical solution.

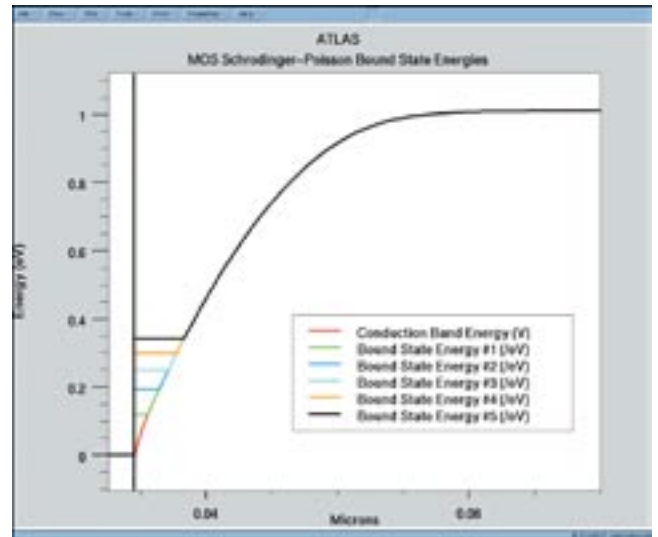


The figure above shows the potential variation of the conduction band edge, as well as the first seven bound state energy levels under the gate of the GaAs/AlGaAs HEMT device. Here we can see that there is confinement due to the heterojunction as well as a potential well due to depletion in the AlGaAs top layer.

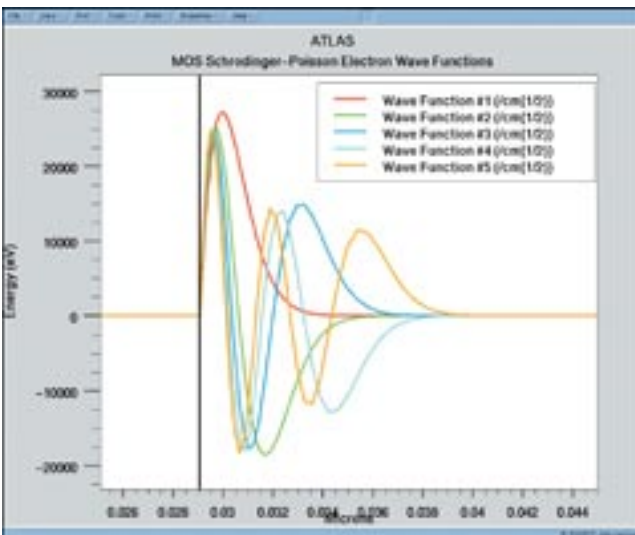




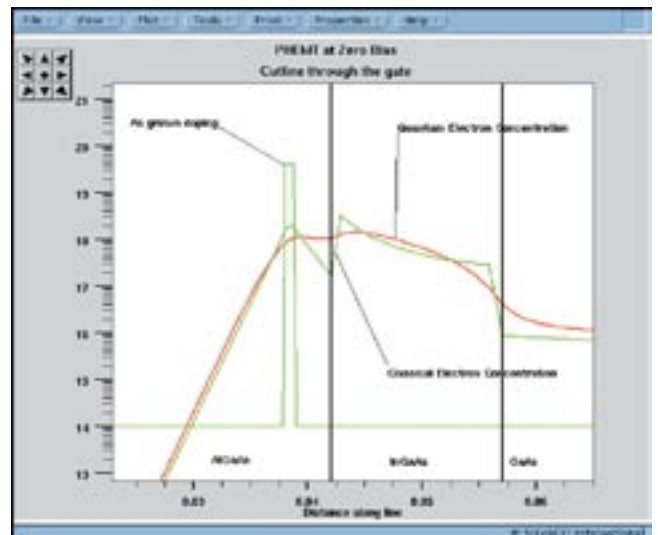
The first seven electron wave functions are shown in the figure above. These wave functions correspond to the the lowest seven bound state energies. These wave functions peak on both sides of the heterojunction due to the potential well created by depletion directly under the gate in the AlGaAs layer.



This figure shows the first five bound state energies under the gate for a thin gate oxide NMOS device in inversion.



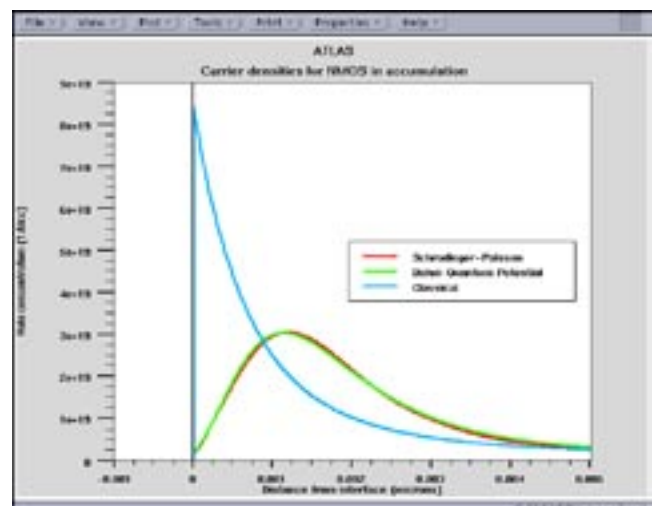
This figure shows the first five electron wave functions under the gate of the NMOS device in inversion.



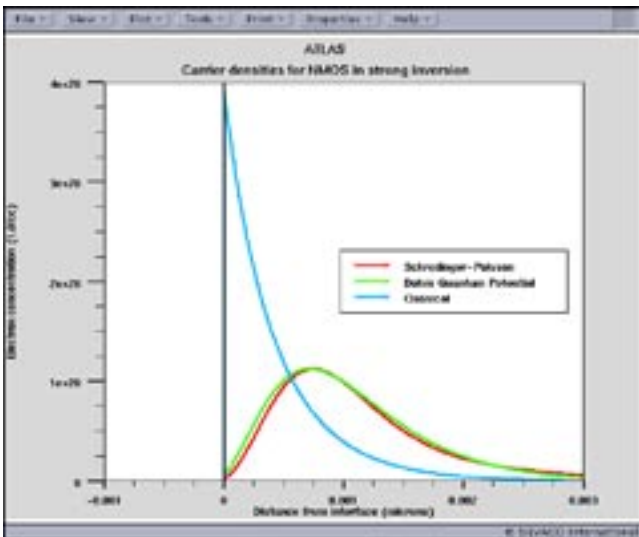
Delta doped PHEMT - cutline through the gate showing smearing of the electron, concentration in the quantum model as compared to classical.

Quantum Moment Transport Models

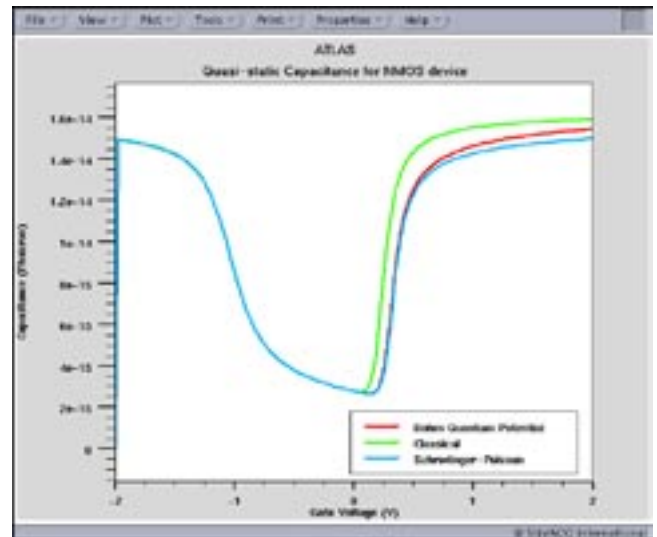
ATLAS has two models for including some of the effects of quantum confinement into the semi-classical drift-diffusion and hydrodynamic carrier transport calculations. The density gradient (DG) method calculates a position dependent potential energy term according to higher derivatives of the carrier densities. The Bohm Quantum Potential (BQP) model calculates a position dependent potential energy term using an auxiliary equation derived from the Bohm interpretation of Quantum mechanics. These extra potential energies then modify the electron or hole distributions. Whilst both methods are derived from pure physics they retain some empiricism, the DG method has one fitting parameter and BQP has two. This flexibility allows the models to approximate well the quantum behaviour of different classes of devices as well as a range of materials. It is possible to get close agreement between Poisson-Schrodinger results and DG or BQP under conditions of negligible current flow. The effects of quantum confinement on the device performance, including I-V characteristics, will then be calculated to a good approximation.



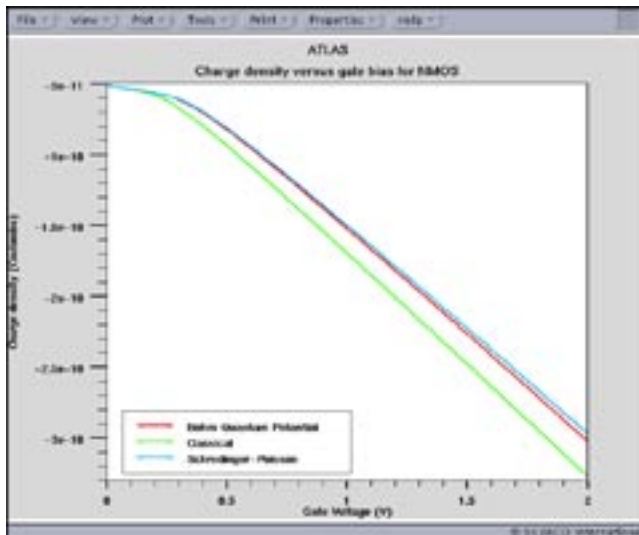
Shows hole concentration under the gate of an NMOS device with a 2 nm thick oxide and uniform p-doping of 1.0×10^{18} /cc. The applied bias of -2 V has put the device into accumulation. The BQP and Schrodinger-Poisson result both show the effect of charge quantisation near the interface.



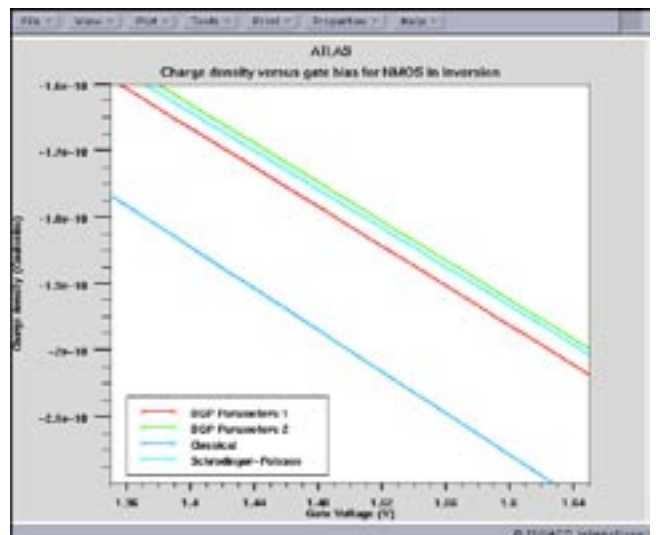
Shows the electron concentration under the gate of an NMOS device with a 2 nm thick oxide. The applied bias of 2 V has put the device in strong inversion. The BQP curve can be made even closer to the S-P curve by a better choice of parameters for the BQP model.



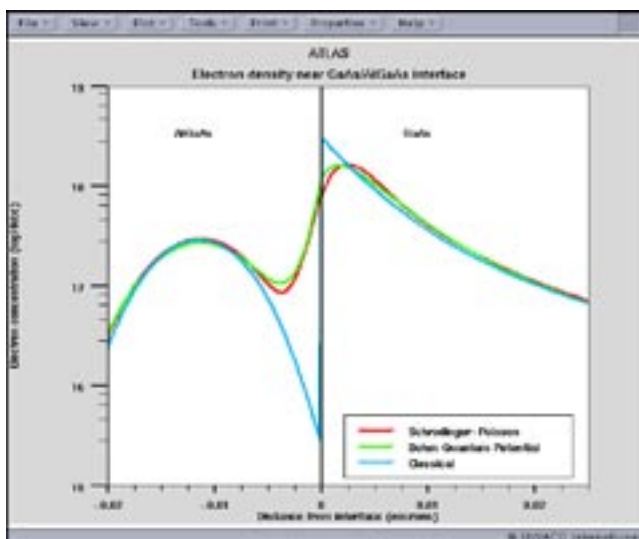
Shows the quasi-static Gate capacitance versus Voltage for the NMOS device. The threshold Voltage for inversion due to quantum confinement is correctly predicted by the BQP and S-P models. Quantum effects are only included for electrons in this figure.



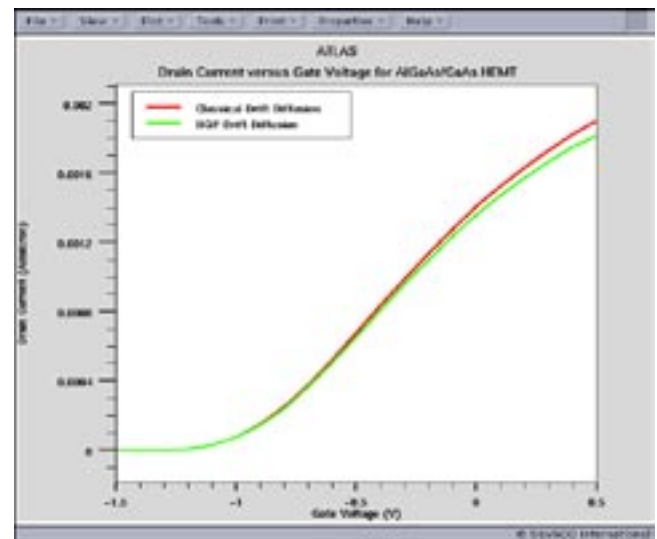
Shows the total electron charge increasing with gate voltage as the NMOS goes into inversion. The BQP and S-P values are similar, and can be made closer to the S-P curve by a better choice of parameters for the BQP model.



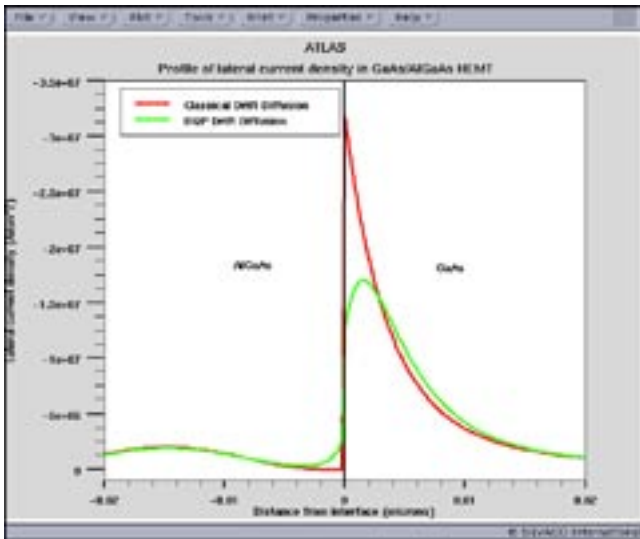
Shows a detail of the curve of charge density (due to electrons) of an NMOS versus gate voltage in strong inversion. In this case two BQP results are shown to illustrate that by choosing the parameters carefully one can get results virtually the same as the Schrodinger-Poisson ones.



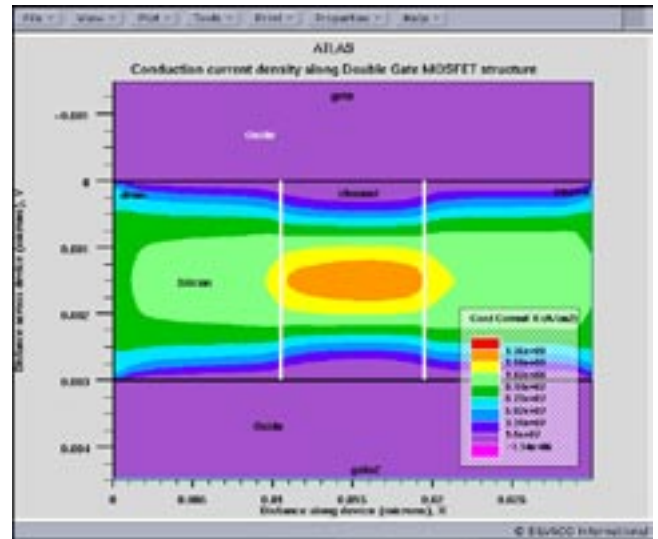
Shows the electron density near the AlGaAs/GaAs interface in the HEMT structure as calculated by Classical, BQP and S-P models.



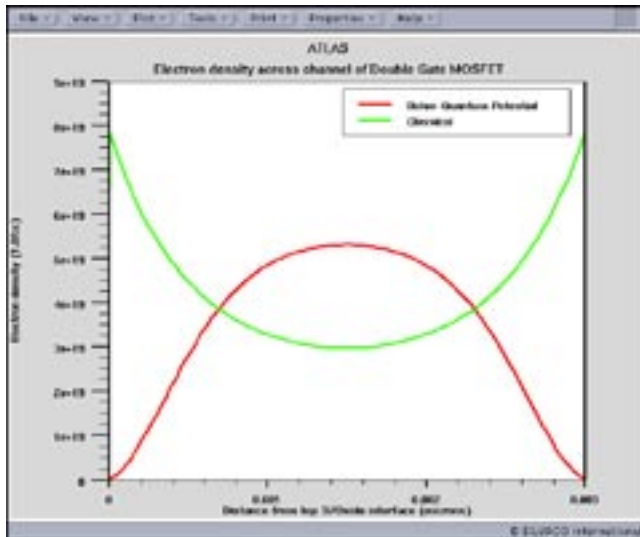
Shows the drain current versus gate bias for the HEMT structure with a drain bias of 0.5 V. The quantum confinement results in a reduced drain current in this case, although this effect will depend on the particular mobility model used.



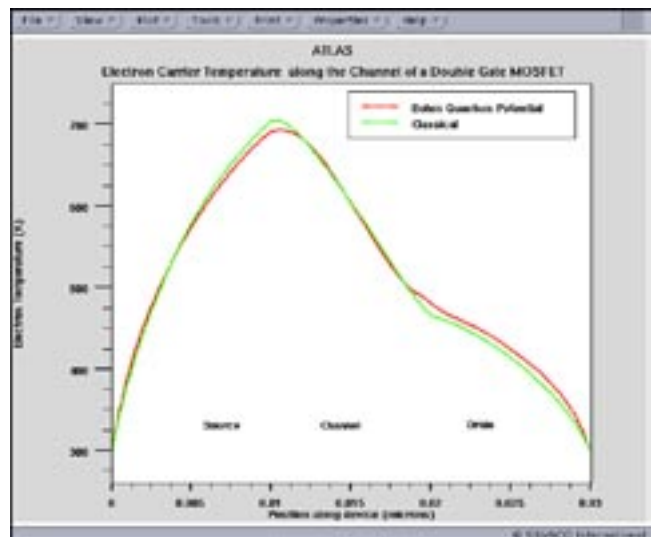
Shows the lateral current density (i.e. parallel to the channel) for the HEMT structure along a line perpendicular to the channel. The drain bias is 0.5 V and the gate bias is 0.5 V. One can see a parallel conduction path in the AlGaAs as well as the quantum model smoothing out the current density in the channel.



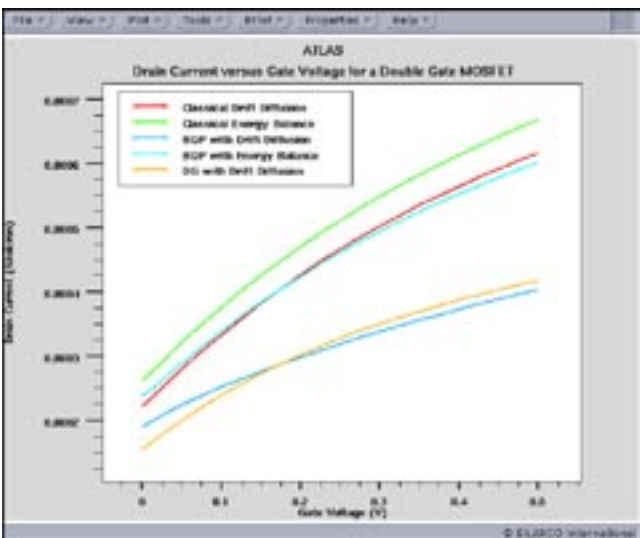
The conduction current density for the Double gate MOSFET at a gate bias of 0.5 V, a Drain bias of 0.5 V. The model used was Bohm Quantum Potential with energy balance. The concentration of the current near the centre of the channel is due to quantum confinement effects



The electron density on a cross-section of the 3 nm wide channel, halfway between the source and drain. The gate bias is 0.5 V, the drain bias is 0.5 V and the carrier temperature at the position of the cross section is approximately 630 K. Quantum confinement effects are pronounced



The electron temperature as obtained using the Energy Balance model for the Double Gate MOSFET structure. The profile is taken along the device between source and drain, that is perpendicular to the section in previous figure. Results for both classical and Bohm Quantum Potential show only a subtle difference in temperature distribution despite the large change in carrier distribution.



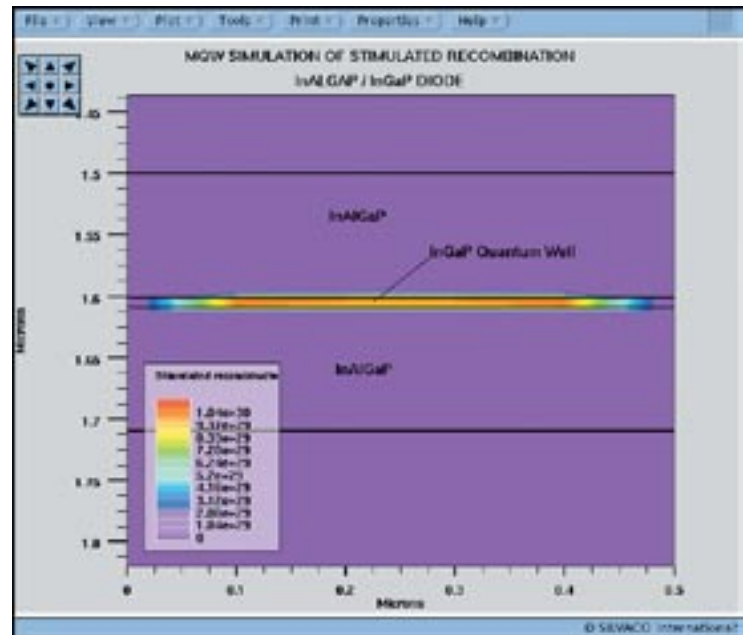
This shows the Drain-Current of a Double Gate MOSFET structure having a channel length of only 10 nanometers. The Gate voltage is applied to both gates which are separated from the 3 nm wide channel by 1.5 nm of oxide. The range of results indicate the importance of choosing the correct model (ie energy balance + quantum effects).

The BQP method is unique to Silvaco. It is available in Quantum2D and in Quantum3D, and for either Maxwell-Boltzmann or Fermi-Dirac carrier statistics. It can be used with solutions of Poisson's equation alone, the Drift-Diffusion equations and the Energy Balance/Hydrodynamic equations.

Multi-Quantum Well (MQW) Model

Simulation of laser diodes requires accurate calculations of spontaneous recombination and optical gain. Two advanced models are available; the Li model, the Chuang model and the Yan model. Both models require information about the bound state energies in each quantum well as well as the bulk momentum matrix element.

ATLAS has included in the Quantum module a method that makes use of a coupled Schrodinger-Poisson method to calculate these terms. Within the quantum well(s) the coupled Schrodinger-Poisson method is used to obtain the bound state energies from the band edge energies and effective masses. Once the bound state energies are known for each well, the bulk momentum matrix element can be calculated. This can then be used to calculate optical recombination as well as local optical gain in the quantum well. Indeed even advanced effects such as whether TE or TM optical modes are dominant, Lorentzian line broadening and even strained layer effects can be accounted for.



Simulation of spontaneous recombination in a quantum well InAlGaP/InGaP/InAlGaP laser diode. The MQW model is used to calculate the recombination in the well.