Simulation of Hot-Electron Effects with Multi-band Semiconductor Devices

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Abstract

The semiconductor industry relies on advanced modeling techniques to develop the next generation of devices. These modeling techniques require numerically solving well established nonlinear differential equations that collectively tell the story of device physics- including equations for electron continuity, hole continuity, and Poisson's equation for electrostatic potential.

In some scaled semiconductor devices and materials, the electric field is high enough to excite electrons and scatter them into higher energy conduction bands. Materials with certain energy band structures are highly susceptible to scattering that can significantly degrade device response. Today's numerical models make use of an empirical relationship between electron velocity and electric field that doesn't handle scattering very well. Modeling is difficult because we do not have a-priori relationships between velocity and field and this need to be developed in advance of numerical solutions for device response.

To understand these issues, we have explored and modeled several additional phenomena, including the Fermi-Dirac integral distribution, multiple band energy levels, and carrier temperature due to heat generation and conduction in the semiconductor lattice, resulting in a more physically-sound approach.

These additions were implemented and demonstrate an increased accuracy in computing quasi-Fermi levels and increased likelihood for convergence as compared to conventional models.

Background- Modeling

Modern Semiconductor device modeling is based on three coupled nonlinear partial differential equations- the Poisson, electron, and hole continuity equations. Many diverse methods have been explored to solve these vital equations [C.S. Rafferty]. This study builds off of a finite element quasi-Fermi (FEQF) modeling approach, which solves for equations in terms of electron and hole quasi-Fermi levels and electrostatic potential [Micheletti, Machek].

$$\nabla^2\Psi = -\frac{q}{\varepsilon}(p - n + N_D - N_A)$$

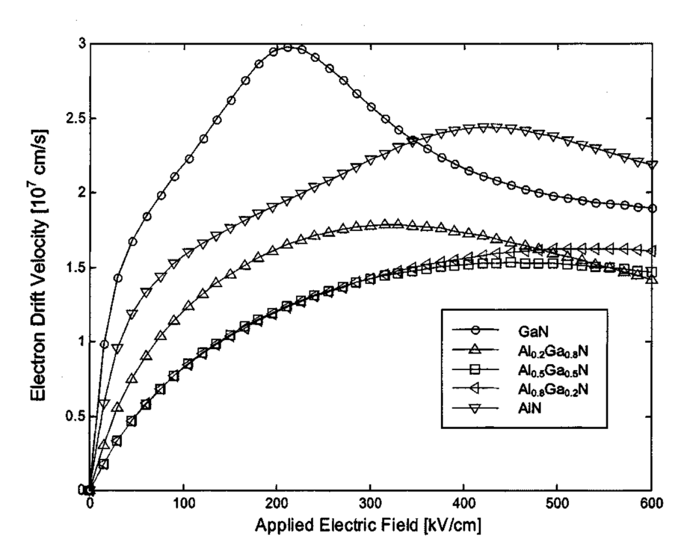
$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot J_n - r_n + g_n \quad \text{and} \quad \frac{\partial p}{\partial t} = \frac{1}{q}\nabla \cdot J_p - r_p + g_p$$

The Poisson, Electron, and Hole continuity equations

Empirical semiconductor models are constructed by using experimental data to tune equation parameters and get a good fit.

The Farahmand [Farahmand] model of transport dynamics for III-nitride compounds is based on a Monte Carlo simulation that includes all of the major scattering mechanisms. The model's parameters are tuned to match experimental data to develop a field dependent mobility relationship for Gallium Nitride (GaN) and other materials.

$$\mu = \frac{\mu_0(T,N) + v^{sat}\frac{E^{n1-1}}{E_c^{n1}}}{1 + a\left(\frac{E}{E_c}\right)^{n_2} + \left(\frac{E}{E_c}\right)^{n_1}}$$



Left: The Farahmand Mobility Equation
Right: The empirical Farahmand Monte Carlo Velocity-Field relationship with tuned parameters

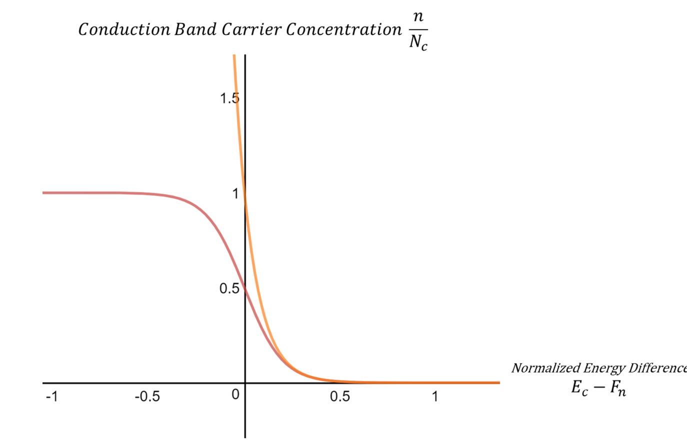
A drawback resulting from experimentally tuned Monte Carlo simulations is the lack of deep physical insights to the system; this method takes a statistical look at the system that glosses over many details of the underlying physics. This leads to convergence issues in simulations of complex devices as well as limited flexibility in tuning for different devices. A more physically rigorous model would allow more physical phenomena to be examined, analyzed, and tuned to build a more reliable model.

This study includes three main additions to the FEQF to increase accuracy in quasi-Fermi computations and decrease the likelihood of convergence issues during computations.

Methods

Model Additions

First, the Fermi-Dirac (F-D) Integral was substituted for Maxwell-Boltzmann distribution for statistical computation of carrier concentrations. Secondly, the new model makes use of the multiple band (multi-band) energy levels of the material to contribute to an increased accuracy of carrier concentrations. Additionally, heat generation and conduction equations are used to compute the temperature of the carriers while keeping the lattice temperature stable. The increased temperature of carriers couples with the multi-band energy levels.



Above: When the quasi-fermi level (F_n) gets near or above the conduction band energy (E_C), the simple Boltzmann model (orange) diverges from the more physically accurate Fermi-Dirac model (red).

Fermi-Dirac (F-D) Integral Statistics

The Fermi-Dirac (F-D) Integral was used to replace the Boltzmann exponential model in calculating the electron concentration for the quasi-Fermi levels. The F-D Integral is most useful in Finite Element Quasi-Fermi (FEQE) analysis because it is dependent on the quasi-Fermi levels and increases the likelihood of convergence.

In order to define the F-D Integral, accurate short series approximations were implemented from P. Van Halen and D. L. Pulfrey, whose methods proved to have an error better than 10^{-5} and can easily be used on a desktop computer.

Boltzmann Statistics

$$n = N_C \exp\left(\frac{E_F - E_C}{kT}\right)$$

$$\Downarrow$$

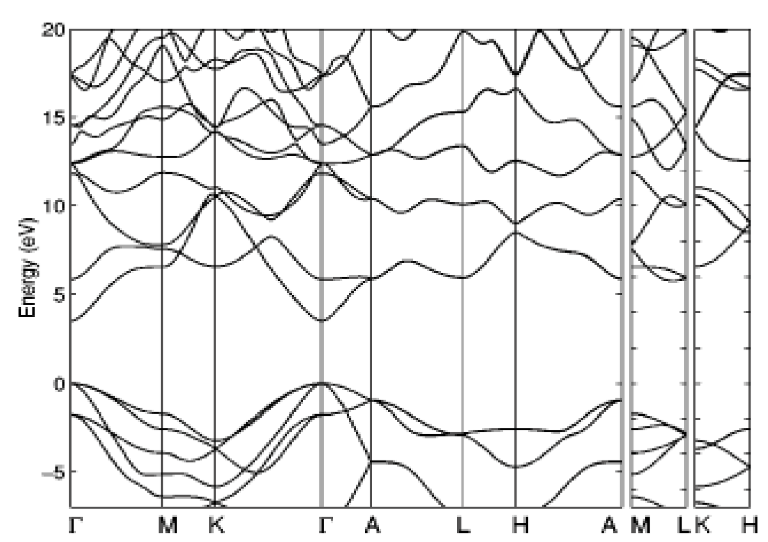
Fermi-Dirac Statistics

$$n = N_C \mathscr{F}_{1/2}\left(\frac{E_F - EC}{kT}\right)$$

Multiple Energy Bands

Accounting for secondary or even trinary energy bands can be important for radiation hard electronics. In cases where ions are excited in higher energy bands, these carriers will be excited and contribute to current flow.

The two major factors that contribute to higher energy band carriers are the electric field strength and carrier temperature. A strong electric field gives some carriers enough energy to jump up to the higher conduction bands whereas heating due to scattering events can also give carriers that extra boost needed to reside in the higher conduction band (as accounted for in the F-D statistics).



Band structure of GaN [Farahmand]

Right: Fermi-Dirac equations implemented for conduction band carrier concentration calculations.

$$n_1 = N_{c1} * \mathscr{F}_{1/2}\left(\frac{E_{fn} - E_c}{kT_{elec}}\right)$$

$$n_2 = N_{c2} * \mathscr{F}_{1/2}\left(\frac{E_{fn} - E_c - dE_{1/2}}{kT_{elec}}\right),$$

where $dE_{1/2}$ is the energy difference between the two lowest conduction band minimums

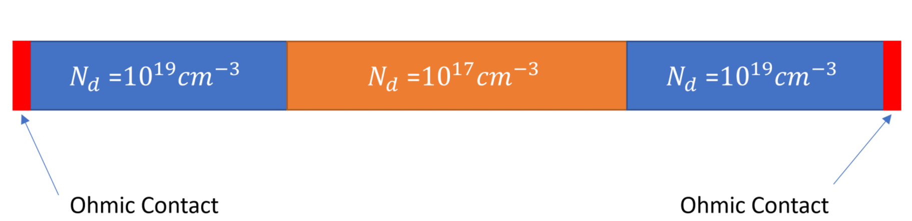
FLOODS

Transient simulation of the models on test structures is carried out using the FLorida Object Oriented Device (FLOODS). FLOODS is a Technology Computer Aided Design (TCAD) tool that discretizes and solves the previously described set of partial and ordinary differential equations on a mesh using the Finite Element Method (FEM).

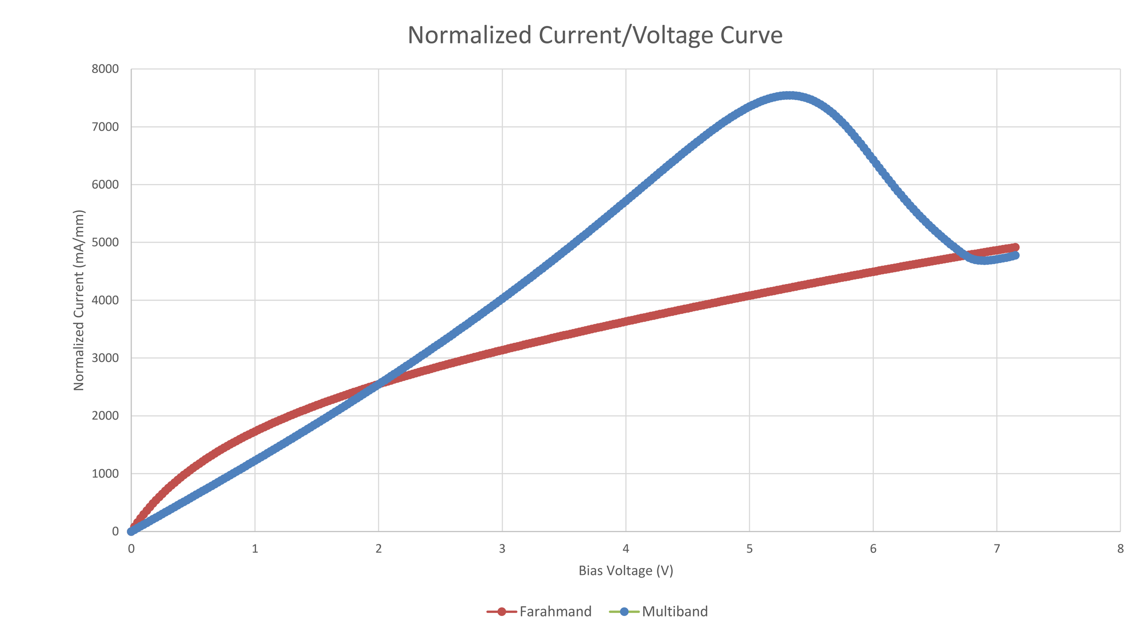
Test Structure

The modeling techniques developed were simulated on a simple resistive test structure. A 1D GaN resistor was used as canvases for simulation of the new modeling techniques.

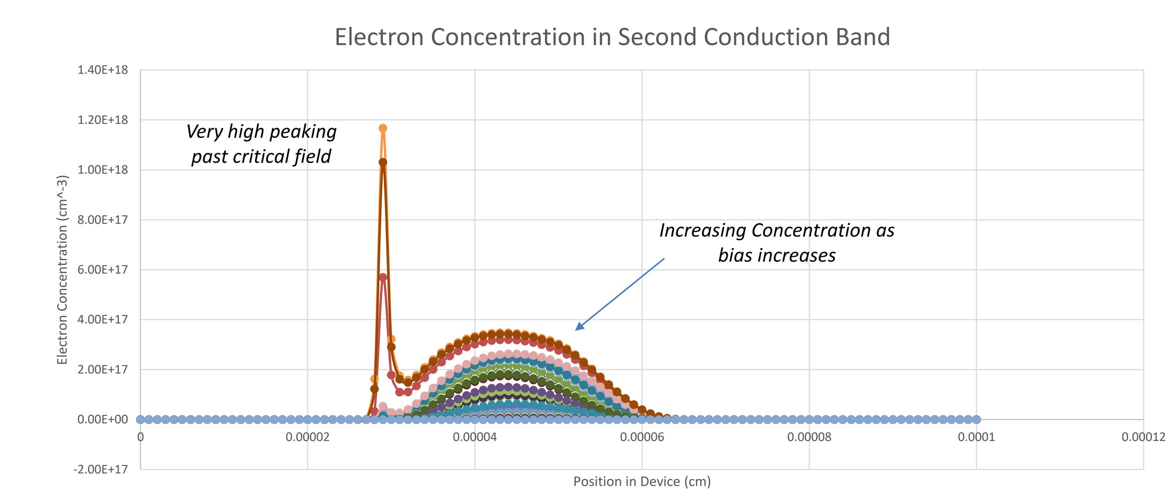
A 1D GaN-based n+/n/n+ resistor was created in FLOODS as a way to analyze the effects of the models in an effort to minimize device structure complexities obscuring results.



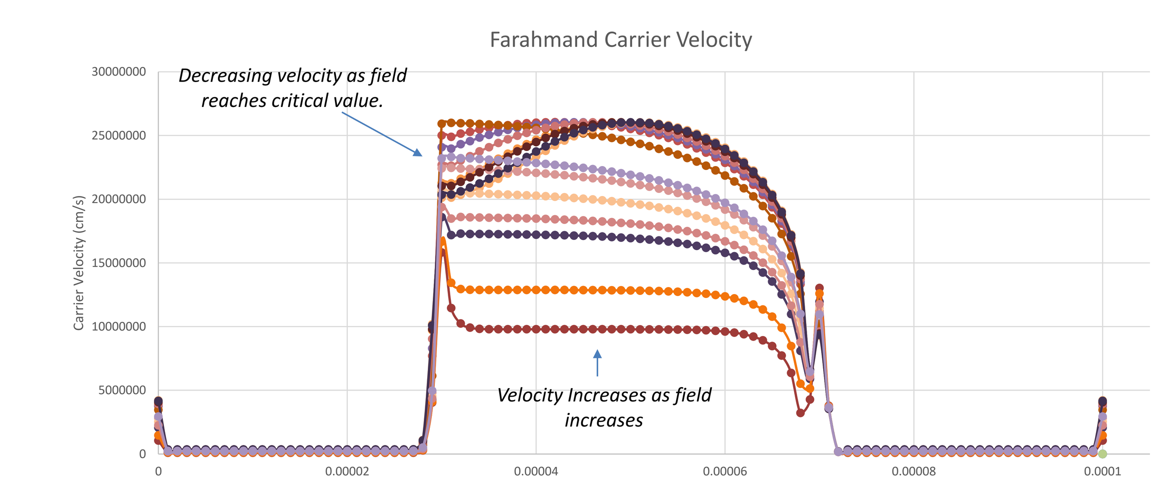
Key Simulation Results



Current-Voltage relationships measured with both models. Notice that the multiband model (blue) clearly shows a roll-over effect, while the Farahmand model (red) lacks a roll-over effect.



Electron Concentration in the second conduction band. The concentration increases as bias increases. The concentration "hump" starts becoming quite appreciable around the critical electric field where roll-off occurs. The peak on the left rises rapidly as the IV rollover completes at around 6/7 V bias.



Carrier Velocity resulting from the Empirical Farahmand model. A significant decrease in carrier velocity begins to occur at around 6V bias, as seen at the upper left corner of the plot where the slope changes from negative to positive. However, this is not enough to cause a rollover in the current.

Key Trends Identified in Simulation Trials

- Current rollover in 2 valley model due to reduced mobility from scattering into the upper conduction bands.
- Current rollover position and width highly dependent on carrier relaxation constant, tau.
- Not seeing rollover in Farahmand model due to the nonlinear response of the device. Rather, a simpler velocity saturation effect is seen.
- Carrier velocity in Farahmand model decreasing in certain parts of the device, but increasing in others.

Future Work

Presently, the device response to applied electric field is being investigated so that an accurate benchmark of the multiband modeling techniques can be obtained. Future simulation studies will include experiments to better understand overall current flux and fine tuning of the multiband model's parameters so that it will perform reliably on a variety of devices.