New Thermionic Emission and Tunneling Models in *ATLAS*

Introduction

In order to simulate heterojunction devices accurately, both the thermionic emission and tunneling mechanisms must be considered when calculating transport across hetrojunctions. Drift-diffusion descriptions of carrier mobility are incomplete at abrupt heterointerfaces. New thermionic emission and tunneling models have been incorporated into ***ATLAS***. This paper discusses the models and presents two examples of device simulation.

Descriptions of the thermionic emission and tunneling across a heterointerface were presented by Yang et al.[1] They developed a thermionic-field emission boundary condition based on the WKB approximation. These models for thermionic emission and thermionic-field emission (tunneling) across a heterointerface have been incorporated into ***ATLAS***.

Current-voltage characteristics for two devices are analyzed as a function of doping, composition and temperature and are compared to data in [1].

nN Heterojunction Device

Carrier transport in an isotype nN heterojuction device is presented. Current due to thermionic emission is significant for nN isotype heterojunctions. These devices show rectifying current vs. voltage characteristics. In reverse bias mode, these devices show varying levels of thermionic emission and tunneling current.

A one-dimensional device was simulated by ***ATLAS***. One region consisted of GaAs with uniform 1e15 /cm^3 n-type dopant, and the second region consisted of $Al_{0.25}Ga_{0.75}As$, with uniform n-type dopant. Three cases were studied, varying the level of uniform doping in the second region. The three values of n-type doping in the second region were 1e15, 1e16 and 5e16 /cm^3. The calculated conduction band profiles under a bias of -0.1 V applied to the first region are shown in Figure 1.

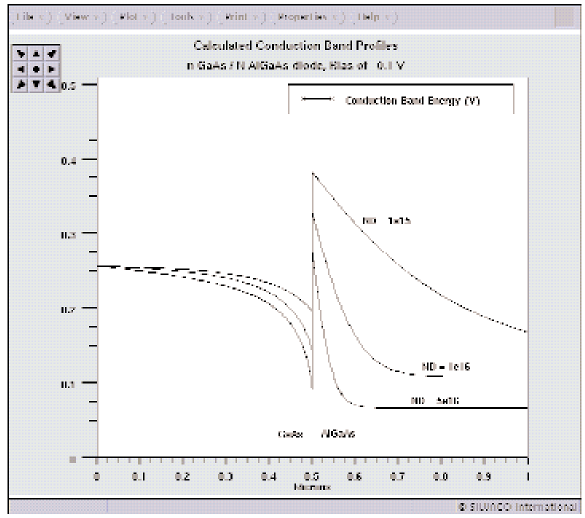

Figure 1: Calculated Conduction Band Profiles for a heterojunction at -0.1V.

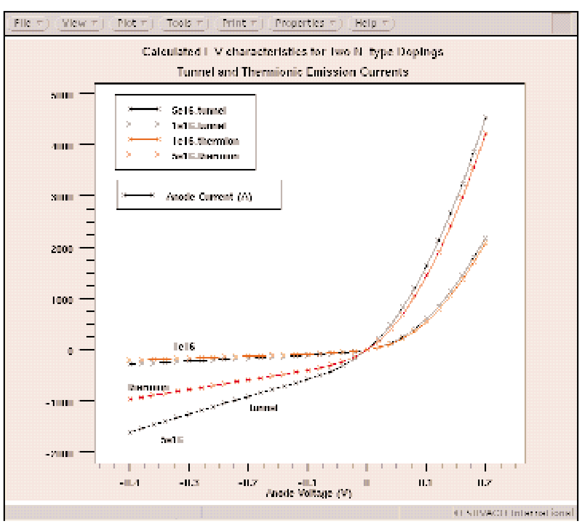

Figure 2: Calculated I-V characteristics of an n-GaAs / n-AlGaAs diode. Units of current are Amps/cm^2.

In the forward bias condition, the conduction band edge of the second region (AlGaAs) is shifted upward, more electrons go over the barrier, hence increasing the thermionic emission. In the reverse bias condition, the electrons injected from the first region (GaAs) see an abrupt energy barrier whose height is determined by the conduction band discontinuity. At higher doping densities, the peak of the conduction band approaches the Fermi level and the energy barrier becomes thinner. The increase of reverse current with increasing n-type doping in the AlGaAs predicted by the thermionic emission model can described by the lowering of the effective barrier height, hence more electrons going over the barrier. However, as the barrier thickness is reduced, the electrons with lower energy than the barrier contributes to the tunneling current. The I-V characteristics are shown in Figure 2. Units of current are Amps/cm^2.

Additional simulation of a pN device was performed. The current density in both forward and reverse bias conditions as a function of n-type doping was simulated. The dominant mechanism for transport was also thermionic emission. (The results are not shown.)

$Al_xGa_{1-x}As$ Graded Heterojunction Barrier

The current transport of a graded isotype heterojunction barrier was studied and simulation results were compared to experimental measurements. The device consisted of

GaAs - $Al_xGa_{1-x}As$ - GaAs regions, all n-type. The GaAs regions were each 0.25 um thick, and the AlGaAs region was 0.078 um thick. The fractional aluminum composition was linearly graded from 0.3 to zero.

The conduction band profiles of the AlGaAs graded heterojunction barrier diode using the thermionic-field emission (tunneling) model at two biases are shown in Figure 3. In the forward bias case, the electrons are injected from region 3 to region 1 and the barrier height is reduced as the conduction band edge of region 3 moves upward. However, in the reverse bias case, the electrons from region 1 encounter an abrupt energy barrier. The electron transport across the barrier occurs either by thermionic emission over the barrier or by tunneling through it. Since the electron energy barrier becomes more transparent under reverse bias, the tunneling process is expected to dominate as the reverse bias increases.

Simulation and experimental measurements confirm that tunneling becomes the predominant mechanism for electron transport across the barrier in reverse bias. Figure 4 shows the forward and reverse bias current in this device at 300K. The calculated results of both the thermionic emission and tunneling currents are shown. These results follow the trend of experimental results. The predicted I-V rectifying properties of this device are observable.

The calculated results of both the thermionic emission and tunneling currents are shown at two temperatures in Figure 5. There is good agreement between the trend of the tunneling simulation and experimental results. Similar to the nN case, the thermionic emission model significantly underestimates the reverse bias current density and tunneling becomes a dominant conduction process.

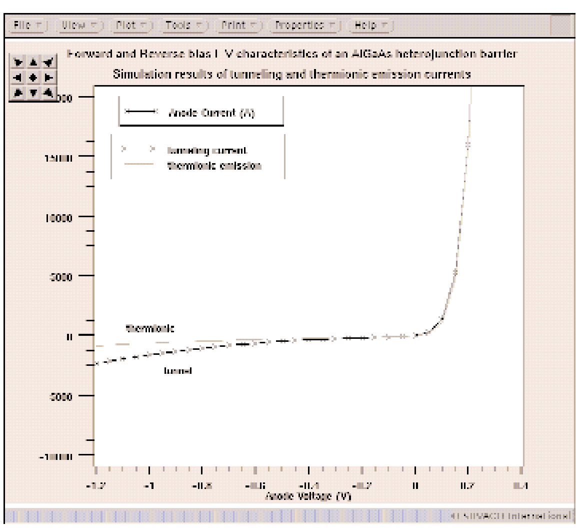

Figure 4: The I-V characteristics of an AlGaAs triangular heterojunction barrier diode at 300K. The calculated thermionic emission current (line) and tunneling current (line and crosses) are both shown.

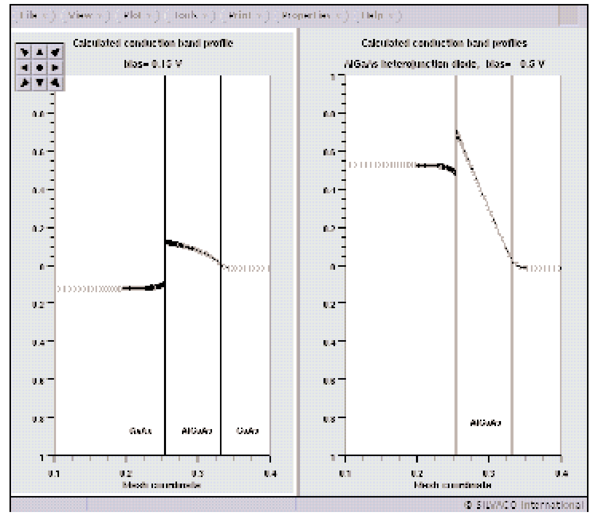

Figure 3: Calculated conduction band profiles of a GaAs - AlGaAs - GaAs diode at bias of a) 0.15 V and b) -0.5V.

Conclusion

New thermionic emission and tunneling models have been incorporated into ***ATLAS***. These models are necessary to simulate heterojunction transport accurately. Simulations of nN GaAs-AlGaAs and isotype graded GaAs-AlGaAs-GaAs heterojunction barriers were presented and compared to published data.

Reference

[1] "Numerical Modeling of Abrupt Heterojunctions Using a Thermionic-Field Emission Boundary Condition", K. Yang, J.R. East and G.I. Haddad, Solid State Electronics, vol. 36, no. 3, pp321-330, 1993].

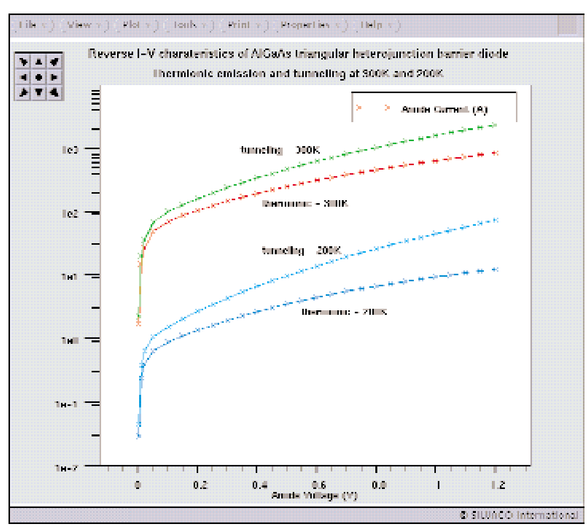

Figure 5: Reverse Bias I-V characteristics at 300K and 200K of thermionic emission and tunneling currents for a graded isotype GaAs-AlGaAs barrier.