

High Field Electron Transport In AlN And AlGaN Semiconductors

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Abstract

An ensemble Monte Carlo simulation is used to compare high field electron transport in bulk AlN and AlGaN. For all materials, we find that electron velocity overshoot only occurs when the electric field is increased to a value above a certain critical field. This critical field is strongly dependent on the material parameters. Transient velocity overshoot has also been simulated, with the sudden application of fields up to 1000 kV/m, appropriate to the gate-drain fields expected within an operational field effect transistor. The electron drift velocity relaxes to the saturation value of 10^5 m/s within 3 ps, for all crystal structures. The steady state and transient velocity overshoot characteristics are in fair agreement with other recent calculations.

Keywords-: Ensemble Monte Carlo, transient, Overshoot, drift velocity.

I. INTRODUCTION

AlN, and its related ternary compounds involving Al and In, have received much attention over the past years because of several new applications, including blue light-emitting diodes (LEDs), blue laser diodes (LDs) [1], and high-power microwave transistors [2-3]. However, one of the biggest problems to overcome has been the lack of a lattice-matched substrate, since bulk group III nitride semiconductors are very difficult to grow in large sizes [4-5]. The large band gap energy of the III-nitrides insures that the breakdown electric field strength of these materials is much larger than that of either Si or GaAs [6-7], enabling, at least in principle, much higher maximum output power delivery in power transistors. Additionally, it has been found that at least the binary compounds, AlN and InN, have higher electron saturation drift velocities and lower dielectric constants that can lead to higher frequency performance of devices made from these materials [8-9].

III-nitrides have a region of negative differential (NDR) conductivity. The mechanism which provides for bulk negative differential resistance is a field induced hot electron transfer from a low energy, high mobility conduction band minimum to a higher energy, low mobility satellite valley. In addition, to observe NDR in bulk semiconductors, a well-defined threshold field as well as sufficiently large intervalley separation energy

must exist. Different separation energies are predicted to give different NDR characteristics, thus providing a degree of engineering freedom in the design of real-space microwave oscillators [5-9]. The experimental determination of the peak electron velocity in a device which exhibits NDR is difficult since dipole domain formation disturbs the uniform carrier concentration needed to determine the carrier velocities. Consequently much of the information available on the peak electron velocity and threshold field is obtained using theoretical methods, particularly those based on Monte Carlo calculations. The Monte Carlo results are only as reliable as the input material parameters used in the simulation which are typically not all known with sharp precision. In order to use Monte Carlo techniques for semiconductor device simulation, it is of principle importance to determine a reliable set of input parameters for each material system studied. In general, one adjusts the lesser known parameters, those not directly measurable, in order to agree with experimental measurements of the velocity-field characteristic. The comparison to experimental measurements, when available, serves as a control on the Monte Carlo calculations. The effects of a particular device geometry on the calculations can then be completely isolated since any difference between the calculated bulk and device quantities must be due solely to the device geometry.

The Monte Carlo method provides an additional advantage in that it can be used as a theoretical laboratory in that parameters can be varied at will and their effects on observables assessed. The method provides a very powerful present herein a series of computer experiments in which the effects of variations in the polar optical phonon energy, dielectric constants, effective masses and central to satellite valley separation energy on the steady-state electron velocity-field relationship for AlGaN are determined [8-11].

The present work studies the high-field transport properties for electrons in bulk GaN and AlGaN in both steady-state and transient situations using ensemble Monte Carlo. It's organized as follows. Details of the simulation model which is used in this work are presented in Sec. II, and results for simulation are interpreted in Sec. III-1 for steady-state and Sec. III-2 for transient situation.

II. SIMULATION MODEL

The ensemble Monte Carlo method used as the basis for this work was developed in Sabzevar and has been used extensively in the study of the electronic properties of many semiconductors and device structures.

At the start of each simulation, ten thousand electron particles are distributed in momentum space according to a 300 K Maxwell-Boltzmann distribution. In the case of the ellipsoidal, non-parabolic conduction valley model, the usual Herring Vogt transformation matrices are used to map carrier momenta into spherical valleys when particles are drifted or scattered. Electrons in bulk material suffer intravalley scattering by polar optical, non-polar optical and acoustic phonons scattering, intervalley phonons, and ionised impurity scattering. Acoustic scattering is assumed elastic and the absorption and emission rates are combined under the equipartition approximation, which is valid for lattice temperatures above 77 K. Elastic ionised impurity scattering is described using the screened Coulomb potential of the Brooks-Herring model. The familiar three-valley approximation of the first conduction band has been used for the zincblende crystal structure of GaN and AlGaIn. Band edge energies, effective masses and non-parabolicities are derived from empirical pseudopotential calculations.

Within the framework of this three valley model, the nonparabolicity of each valley is treated through the application of the Kane model, the energy band corresponding to each valley being assumed to be spherical and is the form of [9-10]:

$$E(k)[1 + \alpha_i E(k)] = \frac{\hbar^2 k^2}{2m^*}$$

where m^* is the electron effective mass in i th valley and α_i is the nonparabolicity coefficient in i th valley.

III. RESULTS

Steady-state electron transport

Figure 1 shows the simulated velocity-field characteristics of AlN and AlGaIn at 300 K, with a background doping concentration of 10^{23} m^{-3} , and with the electric field applied along c -axes. In this figure, the solid circle represent simulation results obtained for AlN and the open circle curves are results obtained for AlGaIn. The simulations suggest that the peak drift velocity for wurtzite AlN and AlGaIn is about $0.9 \times 10^5 \text{ ms}^{-1}$, while that for AlGaIn has no breakdown effect. At higher electric fields, intervalley optical phonon emission dominates, causing the drift velocity to saturate at around $1.1 \times 10^5 \text{ ms}^{-1}$ for AlN.

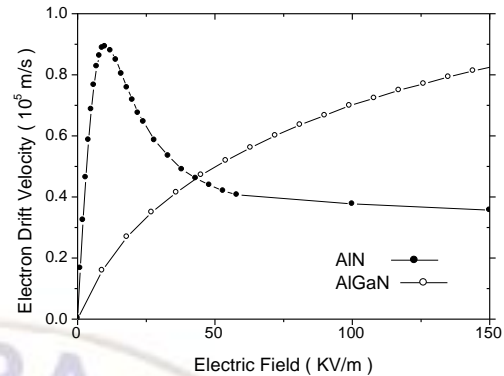


Fig. 1. Calculated velocity-field in wurtzite AlN and AlGaIn at T=300

The calculated drift velocities apparent from figure 1 are fractionally lower than those that have been calculated by other group who assumed an electron effective mass in the upper valleys equal to the free electron mass.

The threshold field for the onset of significant scattering into satellite conduction band valleys is a function of the intervalley separation and the density of electronic states in the satellite valleys. From figure 2, which shows the fractional occupancy of the available valleys as a function of applied field, the threshold fields are found to be $1 \times 10^7 \text{ Vm}^{-1}$ for wurtzite AlN and $1.2 \times 10^7 \text{ Vm}^{-1}$ for AlGaIn.

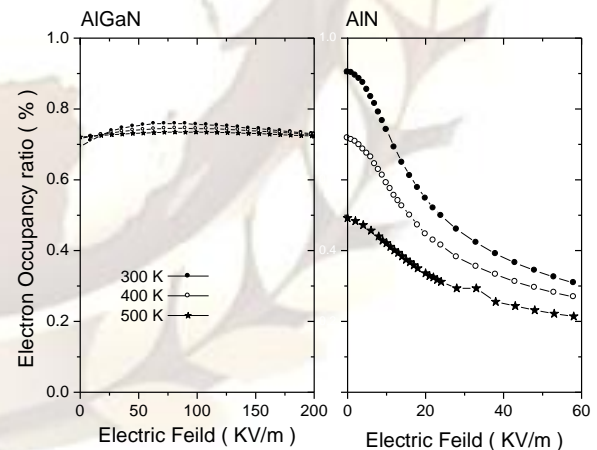


Fig. 2: Fractional occupation of the central Γ valley of wurtzite AlN and AlGaIn as a function of applied electric field using the non-parabolic band model at different temperature.

The average carrier kinetic energy as a function of electric field is shown in figure 3, for lattice temperature up to 500 K. The curves have the S shape typical of III-V compounds, which is a consequence of intervalley transfer. At high fields, the curve for AlN suggests that the average electron

energy is higher than for AlGaN. This difference can be understood By considering the Γ valley occupancy as a function of applied electric field. Intervalley transfer is substantially larger in the AlN than AlGaN phase, due to the combined effect of a lower Γ -valley effective mass, lower satellite valley separation and reduced phonon scattering rate within the Γ -valley, but significant intervalley phonon scattering at a threshold field of $1 \times 10^7 \text{ Vm}^{-1}$.

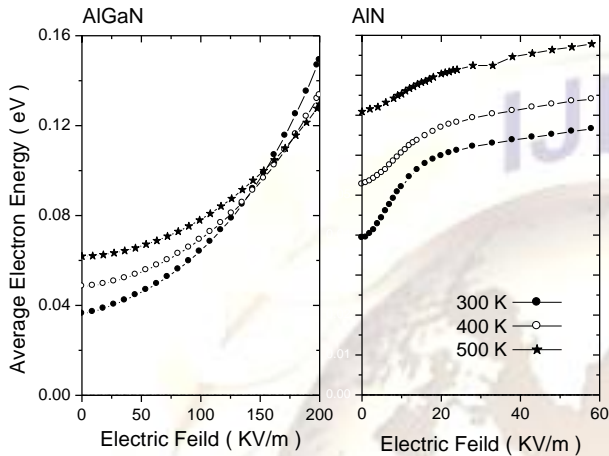


Fig. 3: Average electron kinetic energy as a function of applied electric field in bulk AlN and AlGaN using the non-parabolic band model at different temperatures.

Figure 4 shows the calculated electron drift velocity as a function of electric field strength for temperatures of 300, 450 and 600 K. The decrease in drift mobility with temperature at low fields is due to increased intravalley polar optical phonon scattering whereas the decrease in velocity at higher fields is due to increased intra and intervalley scattering.

It can be seen from the figure that the peak velocity also decreases and moves to higher electric field as the temperature is increased. This is due to the general increase of total scattering rate with temperature, which suppresses the electron energy and reduces the population of the satellite valleys. This latter effect is apparent from the fact that the electron population in the Γ -valley increases with temperature as shown in figure 4.

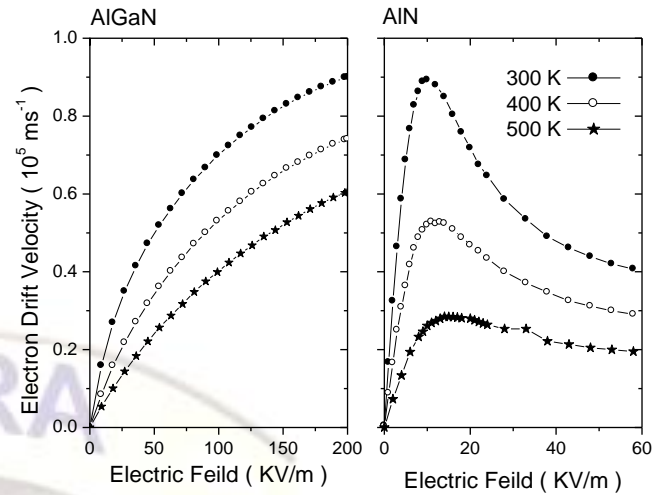


Fig. 4: Calculated electron steady-state drift velocity in bulk AlN and AlGaN as a function of applied electric field at various lattice temperatures and assuming a donor concentration of 10^{23} m^{-3} . The peak drift velocity decreases by about %20 while the threshold field increases by same percent as the lattice temperature increases from 300 to 600 K.

IV. CONCLUSIONS

The computed steady-state electron transport in wurtzite AlN and AlGaN show that, this material has superior electron transport properties. The velocity-field characteristics of the materials show similar trends, reflecting the fact that this semiconductor has satellite valley effective densities of states several times greater than the central gamma-valley. We have also shown that AlN exhibits much more pronounced overshoot effects compared to other nitride materials but at much higher electric fields.

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