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Monte Carlo Simulation of GaN Submicron n^+-n-n^+ Diode with AlGaN Heterojunction Cathode

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Abstract: An ensemble Monte Carlo simulation has been developed to simulate the motion of electrons in a submicron GaN diode with a $Al_xGa_{1-x}N$ heterojunction cathode. It is shown that the hot electron injection through the heterojunction cathode is effective to increase the mean electron velocity of carriers. The analysis has also shown that the mean drift velocity for electrons in the channel is about 2×10^5 m sec^{-1} at bias 4 V. Mean drift velocity in channel decrease with temperature and reach to saturated value about 1.5×10^5 m sec^{-1}.

Key words: Ensemble monte carlo, submicron, heterojunction, drift velocity, channel, Iran

INTRODUCTION

Wide band gap GaN and AlGaN have two main uses in commercial devices providing bright LEDs emitting at Ultraviolet-blue green wavelengths for CD-ROM and sensor applications and heterojunction field effect transistors which can sustain high current densities at elevated temperatures (Besikci *et al*., 2000). It has been shown that GaN has large peak electron velocity and can be an important candidate for high frequency application. A wide energy band gap leads to a low intrinsic carrier concentration which enables a more precies control of free carrier concentration over a wide range of temperatures and hence the devices made of this kind of material will be operable at high temperatures with large breakdown voltage.

Recently, there has been considerable interest in the electron transport in submicron GaN devices for possible high-frequency and high-speed applications. As the transit time of electrons in a device becomes comparable or less than the mean free time between collisions, the electrons will move more or less ballistically in the device and will obtain very high velocities. Simulation of this phenomena in a diode structure have so far only been carried out for a very small anode voltage (Martienssen and Warlimont, 2005) or with rather artificial cathode and anode structures.

However, simulations for higher anode voltages are needed in view of the situation in practical devices where engineering problems call for anode voltages of no less than about the Schottky barrier height or the p-n junction barrier height. The boundary conditions are important as they have significant influence on the space charge limitted current flow which become dominant in submicron devices. In this study we report an ensemble Monte Carlo simulation of the electron transport in a submicron GaN diode with highly doped n^+-layer employed as cathode and anode. The anode voltage applied to the diode ranges from 1-4 V.

SIMULATION MODEL AND RESULTS

An ensamble Monte Carlo simulation have been carried out to simulate the electron transport properties in GaN based diode. The method simulates the motion of charge carriers through the device by following the progress of 10^4 super particles. These particles are propagated classically between collisions according to their velocity, effective mass and the prevailing field. The selection of the propagation time, scattering mechanism and other related quantities is achieved by generating random numbers and using this numbers to select for example, a scattering mechanism. The self-consistent Monte Carlo simulation was performed using an analytical band structure model consisting of five non-parabolic ellipsoidal valleys. The scattering mechanisms considered in the model are acoustic, polar optical, ionized impurity, piezoelectric and nonequivalent inter valley scattering. The nonequivalent inter valley scattering is between the Γ, U and K. Acoustic and piezoelectric scattering are assumed elastic and the absorption and emission rates are combined under the equipartition approximation which is valid for lattice temperatures above 77 K.

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It has been expected that a GaN FET having a submicron and a new ballistic electron injection structure exhibits a high frequency or high speed capability because of the high electron velocity associated with the device structure. Some qualitative analysis has already been reported (Arabshahi *et al.*, 2008). Hence, we have developed a Monte Carlo program which simulates the electron motion in a submicron GaN diode with a $Al_xGa_{1-x}N$ heterojunction cathode, to investigate whether the enhanced ballistic electron injection can directly contribute to a larger mean velocity of carriers. The simulated diode has a n^+-n-n^+ structure with an n-GaN layer (active layer) sandwiched between an n^+-AlGaN layer (cathode) and an n^+-GaN layer (anode). Each layer is 0.15 μm in length and doped abruptly. The doping densities are 10^{22} m^{-3} and 2×10^{23} m^{-3} in the n-layer and n^+-layers, respectively. Aluminium content x for $Al_xGa_{1-x}N$ is varied from 0-0.3. Other parameters used in the present Monte Carlo simulation are the as those used for the earlier simulation on n^+-i(n)-n^+ diodes (Jacoboni and Reggiani, 1983).

We assumed an abrupt heterojunction at the interface between the $Al_xGa_{1-x}N$ and GaN layers. The discontinuity of the conduction band potential ΔE_c is determined as:

$$\Delta E_c = 0.9\,(E_{gx} - E_{go}) \qquad (1)$$

Where, Egx and Ego are the energy gap of AlxGa1-xN and GaN, respectively. The quantum mechanical reflection of electrons associated with the conduction band discontinuity at the interface is also included in the same maner as it was treated by Ridley (1993). Particles crossing one end of the diode are injected from the other end with the velocity distribution cooled to the equilibrium.

Figure 1a and b show the distributions of the electron energy and the electron velocity component parallel to the electric field, respectively. The applied anode voltage is 3 V and the Al content x is 0.2. The solid line in Fig. 1a shows the bottom of the conduction band. Also shown in the same Fig. 1 by broken line is the bottom of the upper valley. The excess energy above the bottom of the conduction band represents the kinetic energy of the lower-valley electrons. There is apparently no upper-valley electron present for this anode voltage. It is seen from the Fig. 1 that in the vicinity of the cathode, the majority of electrons in the active layer have a kinetic energy almost equal to the band discontinuity ΔE_c and a velocity almost equal to the corresponding ballistic one. However, it is also seen that quite a number of electrons have distributed energies and velocities. This tendency becomes even more pronounced with increasing distance from the cathode. This is mainly caused by the polar optical phonon scattering. Some electrons come backscattered from the anode n+-layer. However, the number of such electrons is rather small if the applied voltage Va is not so high as to allow the intervalley transfer of electrons to take place. This was verified by comparing the distribution of Fig. 1a with the one in which all scattering factor are intentionally removed from the active layer. One might suspect why the predominantly forward scatterings by the polar optical phonon disturb the ballistic motion of electrons as shown in Fig. 1. This is due to the low electric field present which is not effective to accelerate the electrons to the forward direction once they are scattered by large angles. The mean electron velocity during transit in the active layer is about 5×10^5 m sec^{-1} in the case of Fig. 1 and it increases to about 6×10^5 m sec^{-1} with the increase of the applied voltage to 5 V as will be shown later.

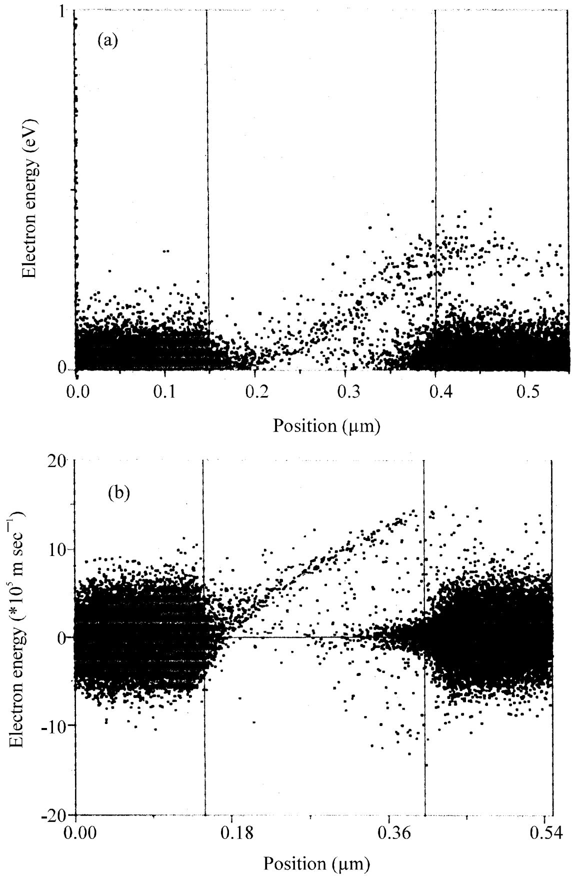

Fig. 1: a) Distribution of electron energy and profile of bottom of conduction band and upper valleys; b) Distribution of component of electron velocity parallel to electric field

Figure 2 shows the current-voltage characteristics of the diodes having a usual n+-GaN Ohmic cathode. It is seen in the Figure 2 that at low applied voltages, the

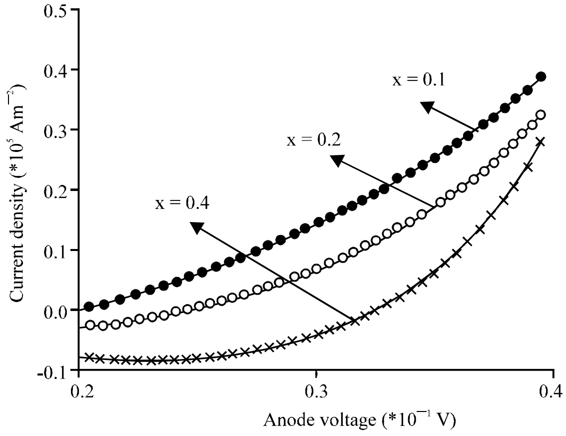

Fig. 2: Current-density versus anode voltage characteristics of diodes having different aluminium content x

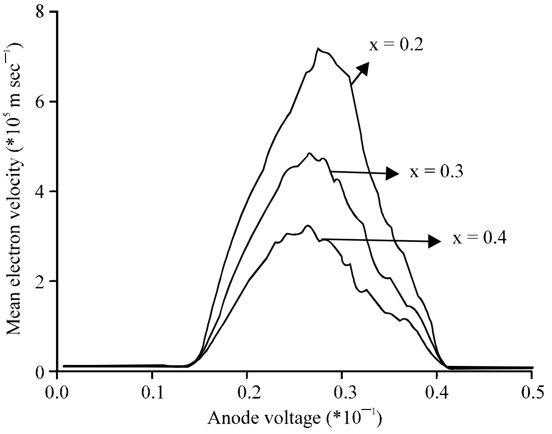

Fig. 3: Mean electron velocity versus anode voltage characteristics of diodes having different aluminium content x

current shows a monotonic decrease with the increase of the Al content. This is due to the fact that the current is mainly limited by the potential barrier associated with the band bending of the $Al_xGa_{1-x}N$ at the heterojunction; the larger the Al content, the larger the potential barrier while at high voltages, the current increases at first and then decreases with the increase of Al content. This is caused by two opposing groups of factors that contribute to control the current. One is that at high anode voltages, the potential barrier at $Al_xGa_{1-x}N$ is negligible for all values of x whereas a higher Al content yields higher initial electron velocities. The other is that the quantum mechanical reflection at the heterojunction increases with increasing x and that a decreasing value of $(V_a-\Delta E_c)$ with increasing x which appears mostly across the active layer has an adverse effect on the acceleration of electrons in the active layer.

In Fig. 3, the mean electron velocities which were evaluated by taking an average of the velocities of all the electrons in the active layer and which may be a more direct Fig. 3 of merit for the logic switching speed or the frequency response of the devices are shown for different Al contents. Within the range of the parameters employed in the present simulation, the mean electron velocity at x = 0.2 shows the highest value of 6×10^5 m sec^{-1} at the anode voltage of 5 V which is about 1.3 times bigger than the highest value for the ohmic electrode. It is seen that the mean electron velocity increases less steeply or even decreases for high anode voltages. This is due partly to the non-parabolicity of the conduction band and partly to the intervalley transfer for electrons taking place when the anode voltage exceeds 4 V.

CONCLUSION

Electron transport in GaN submicron n^+-n-n^+ diode with AlGaN heterojunction cathode has been simulated using an ensemble Monte Carlo simulation. Using Valley models to describe the electronic bandstructure, calculated electron density and potential characteristics show that the intervalley transitions in high electric fields play an important role. The simulation result show also that the mean electron velocity in the active layer is larger than the one with an n^+-GaN cathode if the Al content x is suitably chosen. A large Al content x certainly gives rise to a large initial electron velocity however, it does not directly contribute to a high mean electron velocity if the electric field is not sufficiently strong in the active layer.

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