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Research Note

Ensemble Monte Carlo Simulation of a GaAs n^+-i-n^+ Diode

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In this paper, the results obtained from a one-dimensional Ensemble Monte Carlo simulation of submicron GaAs n^+-i-n^+ diodes under different conditions are presented. To study the electron transport behavior in such structures, the anode voltage and the environment temperature have been set at different values. For active regions of shorter than 0.1 μm and anode voltages of less than 0.29 V, it has been demonstrated that electron transport behavior is quasi-ballistical. For higher anode voltages and longer active regions, intervalley scattering as well as back scattering effects control the electron transport behavior at the anode side of the active region. Next, the n^+-GaAs cathode region is replaced by an n^+-$Al_xGa_{1-x}As$ layer, to study the effects of the hetero-interface on the electron transport behavior. The simulation results illustrate that, in this case, the average velocity profile across the active region is more uniform, however, experiences an overall decrease. Effects of the anode voltage, the Al mole fraction and the active region length on the electron transport behavior are also presented. It has been shown that, by a right selection for these three parameters, one may obtain an optimized profile for the electron average velocity.

INTRODUCTION

The structure of the simulated n^+-i-n^+ diode consists of an undoped layer of GaAs sandwiched between two highly doped layers of n-type GaAs. The undoped layer acts as the active region of the diode while the two highly doped layers play the role of the diode's anode and cathode. The one-dimensional simulation of this diode using a self-consistent method has already been performed [1,2]. In this method, the particle dynamics are first calculated in small time steps, using Ensemble Monte Carlo technique. Then, its potential distribution at the end of each time step is obtained through the use of Poisson equation. Each of the above time steps should be considerably smaller than the inverse of the plasma frequency and the mesh size should also be shorter than the Debye wavelength [3]. The time steps and the mesh size used in this simulation are $\Delta t = 2$ fsec and $\Delta x = 5$ nm, respectively.

The simulator program flowchart is demonstrated in Figure 1. The diode structure, its doping profile and contact regions are defined in "config". Moreover, the particle distributions in the real space and the k-space as well as the potential distribution are initialized in "init". The particle dynamics are next calculated by Ensemble Monte Carlo method in "emc". It is possible that in each time step, some particles reach the contact regions, where they can flow out of the device. Hence, during the simulation, the number of particles may not be constant. For this reason, the number of particles is controlled during each time step. To solve the Poisson equation, one needs to know the carrier density distribution. This distribution is calculated in "charge" with the help of particle distribution, using a method called cloud-in-cell [4]. Finally, the Poisson equation is solved through finite difference method.

Since a discrete vertical n^+-i-n^+ structure is symmetrical and the potential across it varies only in one dimension, there is no need for a two-dimensional simulation for such a structure. However, in a planar structure on which the Ohmic contacts are all located on the same surface, a two-dimensional simulation becomes important. In that case, one can also obtain more information about the carrier distribution throughout the channel depth and length. In this investigation, by varying the anode voltage, the length of the active region and the environment temperature, the carrier transport behavior has been studied

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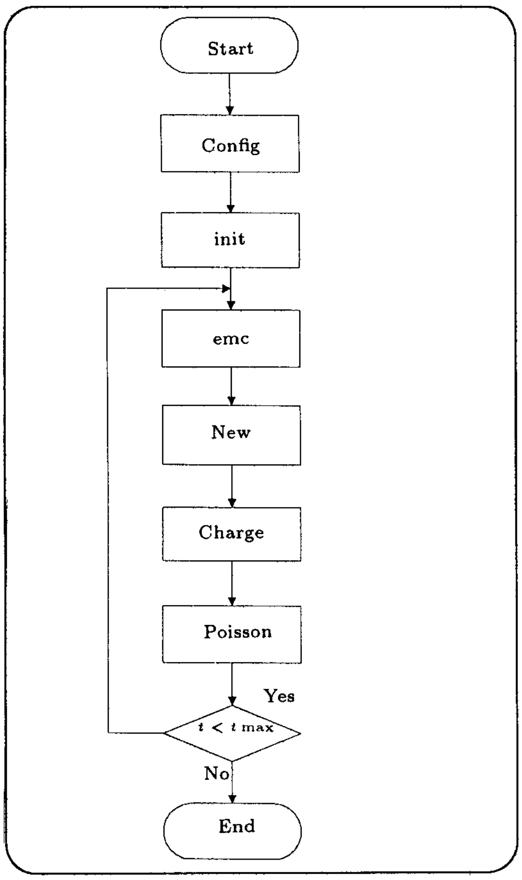

Figure 1. The simulator program flowchart.

using a one-dimensional simulation. Then, the two-dimensional results are presented to show the location of the electrons in a two-dimensional cross section of the device.

Finally, the n^+-GaAs cathode is replaced by a n^+-$Al_xGa_{1-x}As$ layer to investigate the effects of the hetero-interface on the carrier transport characteristics in a heterostructure n^+-i-n^+ diode.

RESULTS AND DISCUSSIONS

In the simulation presented here, the active region length is taken to be 0.25 μm, while the anode and cathode lengths are both equal to 0.15 μm. The doping concentrations in the anode and cathode regions are uniform and equal to 2×10^{17} cm^{-3}. At both ends of the diode, the contacts are Ohmic. For the GaAs, a two-valley (i.e., Γ and L) model is used. The scattering mechanisms used in this calculation are acoustic phonon scattering, polar and non-polar optical phonon scatterings and scattering from ionized impurity atoms.

The potential distribution across the diode for an anode voltage of $V_A = 0.75$ V at $T = 77°$K is illustrated in Figure 2. The electron energy distribution across the diode under similar conditions is depicted in Figure 3. As one can see from this figure, the upper edge of the

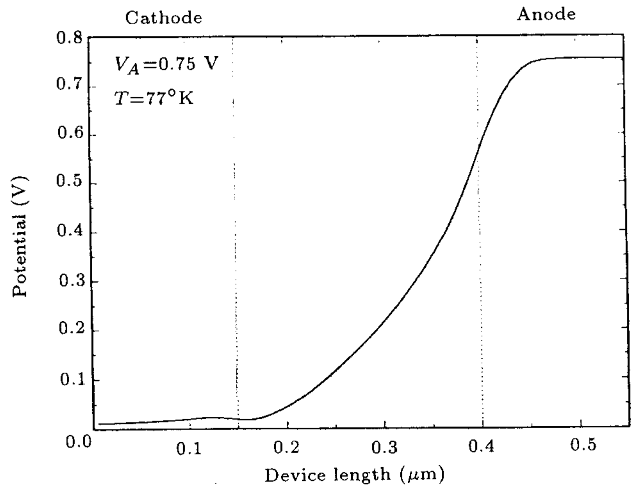

Figure 2. The potential distribution across the GaAs n^+-i-n^+ diode for an anode voltage of $V_A = 0.75$ V at $T = 77°$K.

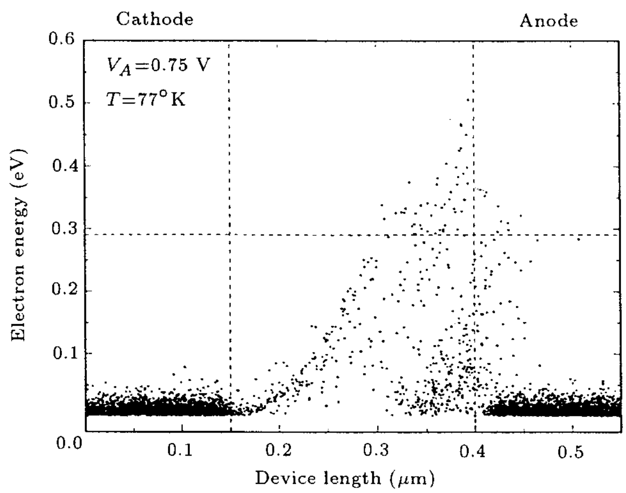

Figure 3. The electron energy distribution across a GaAs n^+-i-n^+ diode, for $V_A = 0.75$ V at $T = 77°$K. The horizontal dashed line shows the energy separation between the Γ and L valleys.

energy distribution envelope moves quasi-ballistically across the active region and is equal to the magnitude of the electronic charge times the potential distribution in that region [5].

As is shown in Figure 4, a similar situation occurs for the electron velocity distribution across the diode under similar conditions. The upper edge of the velocity distribution is an envelope whose velocity is given by:

$$\nu_x = \sqrt{\frac{2qV(x)}{m^*}},$$

where m^* is the effective mass of the electrons in the Γ valley. This also provides that in the active region, the electrons move quasi-ballistically towards the anode.

Figures 3 and 4 show that electrons are accumulated in the neighborhood of the anode in the

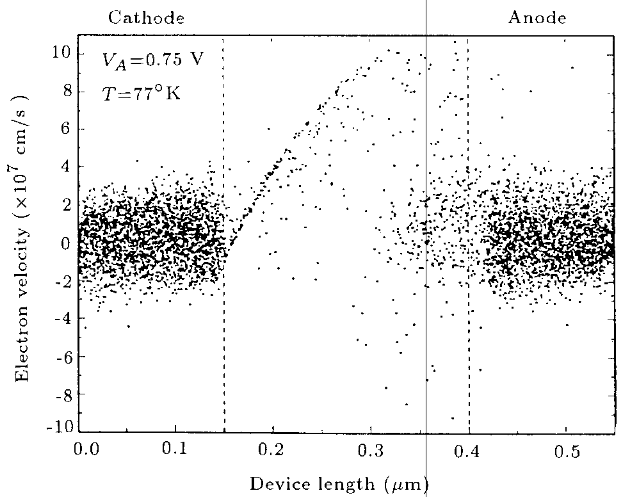

Figure 4. The electron velocity distribution across a GaAs n^+-i-n^+ diode, for V_A = 0.75 V at T = 77°K.

active region. This effect is not due to any of the above mentioned scattering mechanisms in the active region. It occurs because of back scattering from the anode into the active region [1]. As one can see in Figure 3, electrons in the anode have enough energy to move to the L valley. In this valley, carriers scatter in all directions with a high probability. Some of these scattered electrons return to the Γ valley in the active region and result in accumulation of electrons in the vicinity of the anode in that region. To demonstrate this effect more precisely, here the results of a two-dimensional simulation are presented. Figure 5a depicts a two-dimensional distribution for the Γ valley electrons in a cross section of the same diode, for V_A = 0.75 V at T = 77°K. Figure 5b shows a similar distribution for the L valley electrons. As anticipated

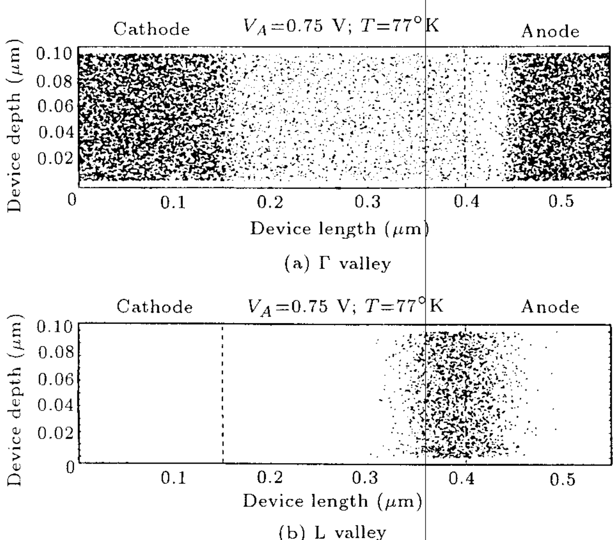

Figure 5. A two-dimensional distribution of electrons in a cross section of a GaAs n^+-i-n^+ diode, for V_A = 0.75 V at T = 77°K: (a) in the Γ valley; (b) in the L valley.

and mentioned before, the distribution along the device depth is almost uniform in both valleys. Profiles for the potential energy, velocity and the electric field resulting from this simulation are also almost uniform along the diode depth and all are nearly similar to those resulting from a one-dimensional simulation. Figure 6 illustrates the electric field profile along the device length as an out come of this two-dimensional simulation. The rise in the electric field just after the cathode in the active region accelerates the electrons in that region. This is the main cause for the quasi-ballistical motion of the electrons in the active region. The high field on the anode side of the diode also justifies population of electrons in the L valley on that side of the diode, shown in Figure 5b.

Changing the anode voltage to V_A = 0.29V which is equivalent to the energy separation between the Γ and L valleys, results in a situation displayed in Figures 7 and 8. These two figures illustrate the electron energy and velocity distribution, respectively. Electrons still move quasi-ballistically in the active region of the diode under the new conditions. They no longer accumulate in the vicinity of the anode in the active region, since, under the new conditions, a few electrons in the anode have enough energy to transfer to the L valley from where the back-scattering to the active region of Γ valley could occur.

Figure 9 compares the average velocity of the electrons across a diode with a 0.25 μm long active region, under three different anode voltages V_A = 0.29, 0.75 and 1.5 V at 77°K. While with an increase in the anode voltage the peak of the average velocity rises, its position in the active region moves towards the cathode, since, in addition to the back scattering effects, more electrons in the vicinity of the anode in the active region gain enough energy to move to the L valley.

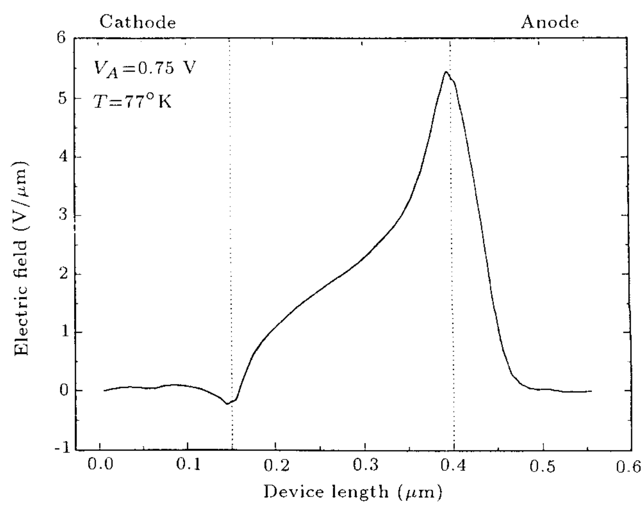

Figure 6. Profile of the electric field along a GaAs n^+-i-n^+ diode, for V_A = 0.75 V at T = 77°K.

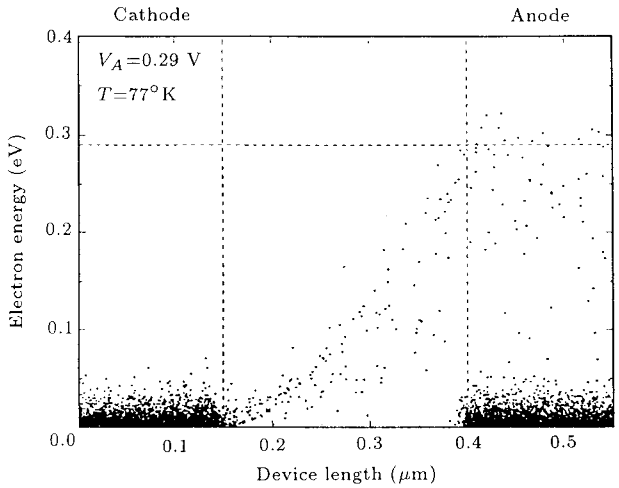

Figure 7. The electron energy distribution across a GaAs n^+-i-n^+ diode, for $V_A = 0.29\ V$ at $T = 77$°K. The horizontal dashed line shows the energy separation between the Γ and L valleys.

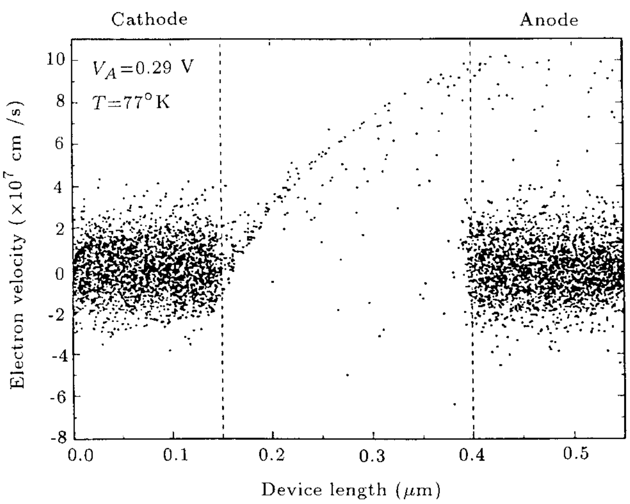

Figure 8. The electron velocity distribution across a GaAs n^+-i-n^+ diode, for $V_A = 0.29\ V$ at $T = 77$°K.

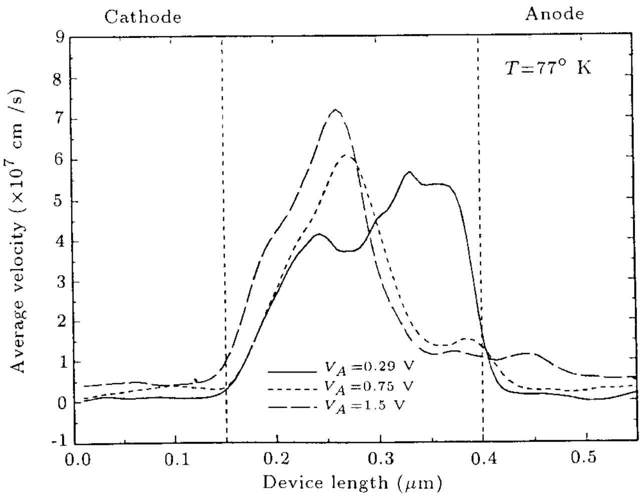

Figure 9. Comparison of the electron average velocity profile across a GaAs n^+-i-n^+ diode, for three different anode voltages $V_A = 0.29$, 0.75 and 1.5 V; at $T = 77$°K.

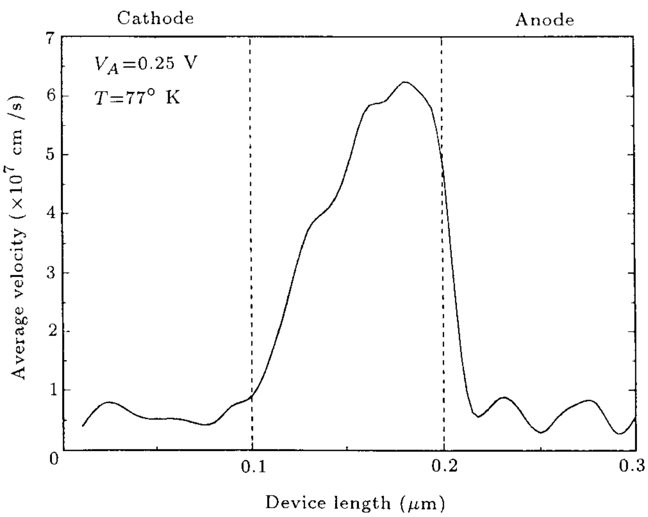

Figure 10. The electron average velocity profile across a GaAs n^+-i-n^+ diode with a 0.1 μm long active region, for $V_A = 0.25\ V$ at $T = 77$°K.

Referring to Figure 7 for $V_A = 0.29\ V$ at $T = 77$°K, one realizes that none of the electrons in the active region are in the L valley, even in the vicinity of the anode. However, as Figure 9 shows the peak of the corresponding average velocity is lower than the peaks corresponding to the higher voltages. This is because for $V_A = 0.29$ V, electron transport near the anode in the active region is dominated by collision processes. Through reducing the active region length, one may almost eliminate this effect. This is demonstrated in Figure 10, in which the average velocity of electrons across a diode with a 0.1 μm long active region is illustrated for $V_A = 0.25$ V at T=77°K. In such an active region, the collision processes have been almost eliminated and the peak in the average velocity has moved very close to the edge of the anode.

Elevating the environmental temperature will result in higher scattering rates. Figure 11 compares the electrons average velocities across a diode with a 0.25 μm long active region for $V_A = 0.75$ V at three different temperatures $T = 77$, 150 and 300°K. At $T = 77$°K, the thermal energy is 7 meV which is much smaller than the energy of the longitudinal POP. Therefore, the POP scattering is dominant at this temperature. On the other hand, due to the relatively high field in the vicinity of the cathode in the active region, the POP scattering rate due to absorption is negligible in comparison with its rate due to emission. Therefore, under such conditions, one expects the electrons to move quasi-ballistically in nearly the first half of the active region. Increasing the temperature towards 300°K, the POP scattering rates due to both absorption and emission increase considerably, so that the electron transport behavior after passing nearly

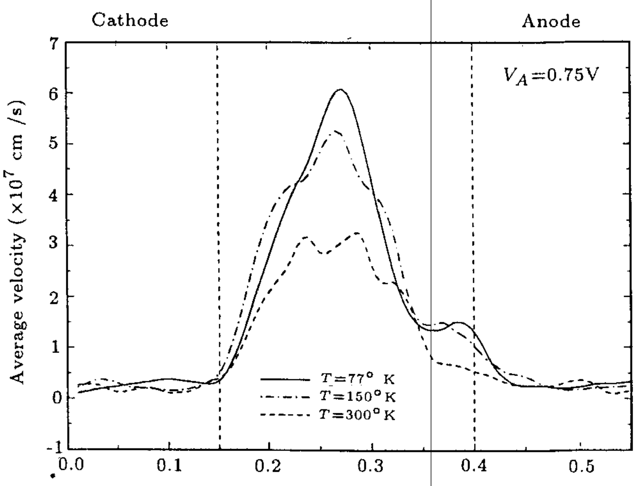

Figure 11. Comparison of the electron average velocity profile across a GaAs n^+-i-n^+ diode, for $V_A = 0.75$ V at three different temperatures $T = 77$, 150 and 300°K.

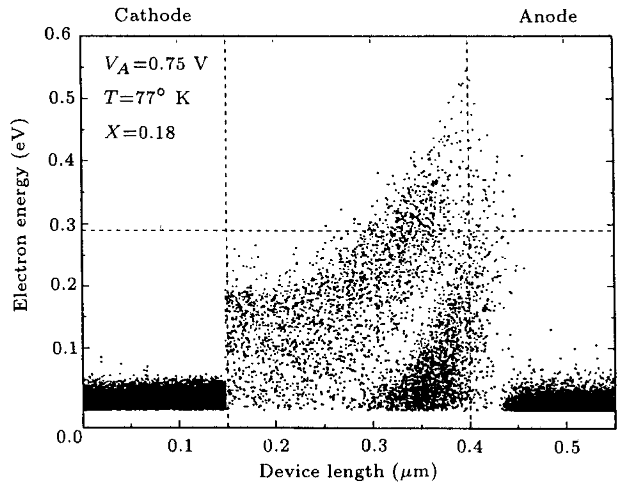

Figure 12. The electron energy distribution across a n^+ ($Al_{0.18}Ga_{0.82}As$)-i (GaAs)-n^+ (GaAs) diode, for $V_A = 0.75$ V at $T = 77$°K. The horizontal dashed line shows the energy separation between the Γ and L valleys.

the first 0.1 μm of the active region becomes collision dominant and it is no longer ballistical, thereafter.

Subsequently, the n^+-GaAs cathode was replaced by an n^+-$Al_xGa_{1-x}As$ layer, to increase the energy of those electrons entering the active region from the cathode. The conduction bandgap discontinuity at the interface, ΔE_C, can play the role of a launching platform for the high energy electrons into the active region. On the other hand, those electrons tending to scatter back into the cathode, from the active region, face a potential barrier at the heterointerface. Therefore, the energetic electrons accumulate in that region, causing an increase in the carrier velocity there. In this model, two additional effects are taken into account: 1) the quantum reflection coefficients for those electrons crossing the hetero-interface and 2) the tunneling of electrons through the spike in the conduction band at the cathode side of the interface. In this case doping concentration of the n^+ anode and cathode are both 5×10^{17} cm^{-3}, while it is 5×10^{14} cm^{-3} for the active region.

Figure 12 depicts the electron energy distribution across a diode in which the Al mole fraction is $x = 0.18$. This distribution is obtained for $V_A = 0.75$ V and $T = 77$°K. In comparison with a conventional n^+-i-n^+ diode, the carriers on the cathode side of the active region in the new structure have relatively high energies. Approaching the anode, in the new diode, more electrons gain enough energy to move to the L valley both in the active region and the anode. Consequently, velocity of the electrons at the anode side of the active region decreases (Figure 13) and, thus, the peak of the average velocity shifts towards the cathode (Figure 14). Figure 13 displays the velocity distribution for the electrons across the above mentioned diode. The upper envelope in the velocity

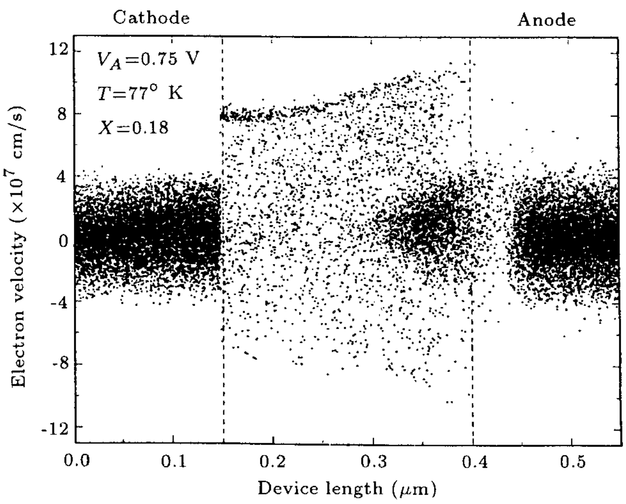

Figure 13. The electron velocity distribution across an n^+ ($Al_{0.18}Ga_{0.82}As$)-i (GaAs)-n^+ (GaAs) diode, for $V_A = 0.75$ V at $T = 77$°K.

distribution, in this case, also demonstrates the quasi-ballistical motion of the electrons.

As discussed before, decreasing the anode voltage may reduce the number of electrons in the L valley and, hence, lowers the back scattering effects. Figure 14 demonstrates the effects of the anode voltage on the average velocity of the electrons across a heterostructure n^+-i-n^+ diode, at $T = 77$°K. As mentioned previously, by reducing the anode voltage from 0.75 V (solid line) to 0.24 V (dashed line), the average velocity increases considerably throughout the active region. By further reduction in the anode voltage, although the average velocity profile across a major portion of the active region remains almost uniform, its peak value decreases. The dotted dashed curve depicts the profile of the average velocity for the electrons across the above mentioned diode for $V_A = 0.14$ V. This

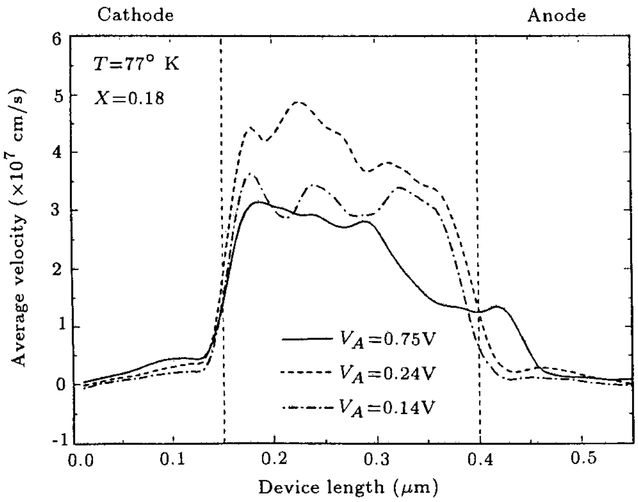

Figure 14. Average velocity of the electrons across an n^+ ($Al_{0.18}Ga_{0.82}As$)-i (GaAs)-n^+ (GaAs) diode, for V_A = 0.14, 0.24 and 0.75 V at T=77°K.

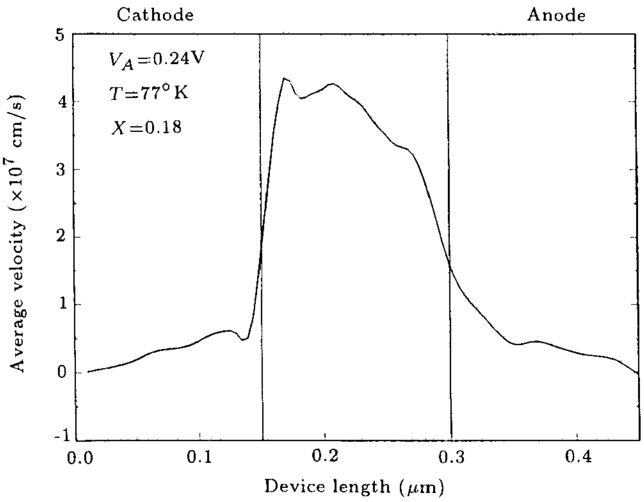

Figure 16. Aerage velocity of the electrons across an n^+ ($Al_{0.18}Ga_{0.82}As$)-i (GaAs)-n^+ (GaAs) diode with a 0.15 μm long active region, for V_A = 0.24 V at T = 77°K.

reduction in the velocity occurs because the electron energy is almost equivalent to the barrier height at the heterointerface.

If one increases the aluminum mole fraction and maintains the anode voltage at a constant value, the electron average velocity on the cathode side of the active region would increase. This is a result of an increase in the electron energy due to the enhanced barrier at the heterointerface. However, another consequence of this energy increase is that some electrons at the anode side of the active region gain enough energy to move to the L valley there. The latter effect and the backscattering from the anode L valley into the active region Γ valley make the profile of the average velocity to fall at anode side of the active region. Figure 15 compares the average velocities for the electrons across two diodes with the Al mole fractions of x = 0.18

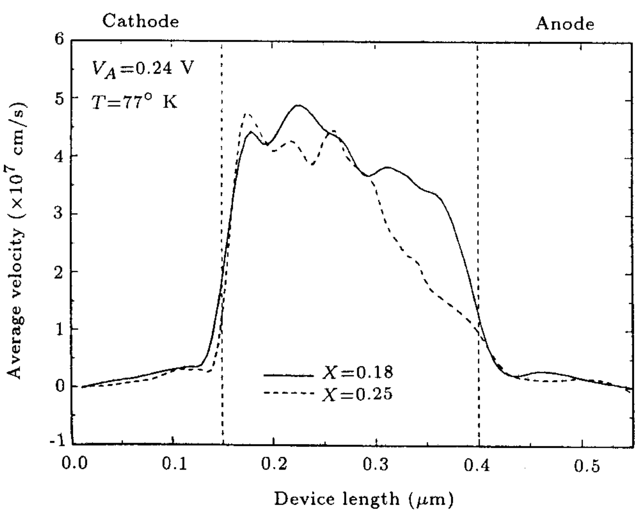

Figure 15. Average velocity of the electrons across two different n^+ ($Al_xGa_{1-x}As$)-i (GaAs)-n^+ (GaAs) diodes, for V_A = 0.24 V at T = 77°K. The Al mole fractions for these two diodes are x = 0.18 and 0.25.

and 0.25, for V_A = 0.24 V at T = 0.77°K. The solid curve demonstrates the result for the device with an n^+-$Al_{0.18}Ga_{0.82}As$ cathode and the dashed curve depicts the result obtained for the diode with an n^+-$Al_{0.25}Ga_{0.75}As$ cathode.

Finally, by reducing the active region length to 0.15 μm, one would expect to see an improvement in the average velocity profile at the anode side of the active region, since in this case, the POP scattering effect is decreased as depicted in Figure 16. A right selection for Al mole fraction, the active region length and the anode voltage results in an optimized profile for the electron average velocity.

CONCLUSIONS

In this paper, it has been demonstrated that motion of electrons in the first 0.1 μm of the active region at a low temperature is quasi-ballistical, when the anode voltage in a GaAs diode is less than 0.29 V. It is also concluded that after the first 0.1 μm in the active region collision processes become dominant for such biasing conditions. This causes the electron average velocity profile to drop below that of the higher voltages. Under higher anode voltages, at a low temperature, back scattering effect becomes important. Hence, under such conditions, electrons accumulate in the vicinity of the anode in the active region. Moreover, it has been illustrated that at high temperatures, for an anode voltage of 0.75 V, POP and backscattering are both significant. These two effects reduce the peak of the average velocity profile considerably.

It has been presumed that by replacing the GaAs cathode with an $Al_xGa_{1-x}As$ layer, higher energy carriers crossing the heterointerface increase the electron velocity on the cathode side of the active region, in the new structure. Decreasing the anode voltage down to a certain value, below the Γ and L valleys energy separation, results in a rise in the average velocity, due to the fact that in this situation the backscattering effect is eliminated and also there is no electron left in the active region Γ valley. For an Al mole fraction of 0.18 at $T = 77°$K, the anode voltage has been reduced to 0.14 V which is almost equivalent to bandgap discontinuity at the heterointerface. In this case, the average velocity profile drops down, however, is almost uniform across the active region. Finally, it has been concluded that a right combination of the Al mole fraction, the active region length and the anode voltage may result in an optimized profile for the electron average velocity.

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