



Comparison of electron transport properties in submicrometer InAs, InP and GaAs $n^+ - i - n^+$ diode using ensemble Monte Carlo simulation

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Abstract

Monte Carlo simulation of electron transport in an InAs and InP diode of $n^+ - i - n^+$ structure is compared with GaAs diode. All of these calculations are performed for the lattice temperature $T=300$ K. We approximate the conduction band of GaAs by taking into account the Γ valley in the center of the first Brillouin zone, four equivalent L valleys and three equivalent X valleys. The anode voltage ranges from 0,75V, 1,5V and 2 V. The distributions of electron energies, electron velocities, potential and the profiles of the electric field are computed. For higher anode voltages and longer active regions, inter-valley scattering as well as back scattering effects control the electron transport behaviour at the anode side of the active region. Also, the effects of the lattice temperature and doping on the length of the active layer are discussed. Our calculations show that electron reach to a higher drift velocity in the InAs than InP and GaAs. So InAs material is a good candidate for high power device fabrication.

Keywords: Monte Carlo simulation, electron energies, electron velocities, equivalent valleys L, Γ , X electron transport in a submicron InP , InAs and GaAs .

1. Introduction

The structure of the simulated $n^+ - i - n^+$ diode consists of an undoped layer of InP/InAs sandwiched between two highly doped layers of n-type InP/InAs. 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 (EMC) [3-4-5]. 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 [6]. The basic steps are the following:

- i) Set up geometry and discretization scheme-two parameters that play an important role in the choice of the time step and the grid size are the plasma frequency and the Debye length [7].
- ii) Charge assignment-the charge of each particle is assigned to a particular mesh point [3]. Since it is not possible to simulate all the electrons present in a real device, each simulated particle represents a cloud of electrons for the purpose of estimating currents, charge, and field distributions. For all other purposes, each individual particle carries its elementary charge e . The doping charge is also added to the mesh according to its distribution.
- iii) Potential solution-Poisson's equation is solved to determine the electrostatic potential at the mesh points. In connection to EMC simulations, a finite difference scheme is generally used.
- iv) Flights-Each particle, now treated as an individual electron, undergoes the standard MC sequence of scatterings and free flights [5], subject to the local field previously determined from the solution of Poisson's equation. The MC sequence is stopped at fixed times, when the field is adjusted following the steps described above. The description of the problem is completed by setting initial and boundary conditions. The initial conditions are not so important, since only the self-consistent steady state result is usually retained. Boundary conditions are instead crucial, in particular in submicrometer devices, where contact properties drastically influence the whole behaviour of the device [8].

In this article, we report an ensemble Monte Carlo simulation of the electron transport in a submicron InP, InAs and GaAs diodes with highly doped n⁺-layer employed as cathode and anode. The diode geometry used in all the simulations has a total length of 0,75µm. The active channel is situated in the middle of the device with a thickness of 0,25 µm. The cathode and anode n⁺-layers of 0,25 µm are highly doped with n⁺ = 2.10¹⁷ cm⁻³, while the ni-region is assumed to be undoped. Hence, the donor density in this layer equals the intrinsic value. Our self-consistent Monte Carlo simulation was also performed using an analytical band structure model consisting of three non-parabolic ellipsoidal valleys. The scattering mechanisms used in this calculation are acoustic phonon scattering, polar and non-polar optical phonon scattering, inter-valley scattering and scattering from ionized impurity atoms. We will focus our simulations on this device considered at room temperature with 0,75V, 1,5V and 2 V applied bias.

2. Results and Discussions

Fig.1 shows the simulated velocity-field characteristics of Zinc blende GaAs, InP and InAs semiconductors at 300 K, with a background doping concentration of 10¹⁷ cm⁻³. The simulations suggest that the peak drift velocity for GaAs is as high as ~ 2,3.10⁷cm.s⁻¹, while that for InP is about ~ 2,5.10⁷cm.s⁻¹ and InAs is about ~ 3,22.10⁷cm.s⁻¹. At higher electric fields, intervalley optical phonon emission dominates, causing the drift velocity to saturate at around 1.10⁷cm.s⁻¹ for all materials.

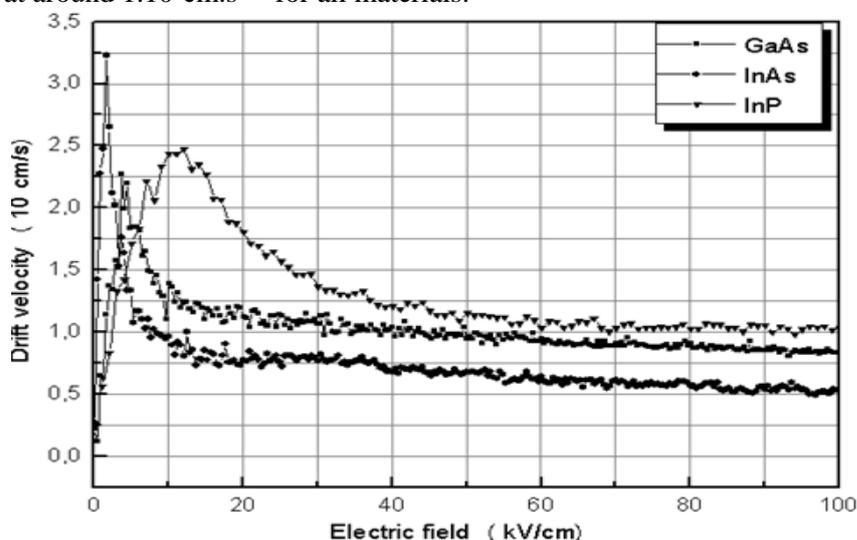


Figure 1: Calculated steady-state electron drift velocity in bulk zinc blende InAs, InP and GaAs at room temperature.

Fig. 2 and Fig. 3 show that electrons are accumulated in neighbourhood of the anode in the active region. As discussed in [9], this accumulation is not a result of the scattering in the active layer, but it is caused by the back-scattering of electrons from the anode n⁺-layer. The back-scattering of these electrons takes place, since the electrons which move almost ballistically through the active layer gain high enough energies to enter the L-valleys in the n⁺ anode layer, where they are scattered isotropically with high scattering probabilities and are subsequently retransferred to the Γ valley. A great portion of these just created Γ electrons possesses a component of the wave vector in direction towards the ni-layer and, therefore, are able to reenter the active layer. We note that the maximum value of the drift velocity reached in the active layer exceeds the maximum stationary-state bulk velocity greatly for both VA=0,75V, 1,5 V and 2 V (Fig.4). Thus, ballistic transport plays an important role in the considered device [10-11].

Fig. 2 compares the average velocity of the electron across a diode with an active region of 0.25 µm for anode voltage VA=0.75V, 1.5V and 2V at 300 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 (Fig.3). The electrons velocity in InAs diode is more than InP and GaAs (12.10⁷ cm.s⁻¹ in InAs, in InP 4,8. 10⁷ cm.s⁻¹ and 7,43. 10⁷ cm.s⁻¹ in GaAs) in the same voltage. It is partly due to heavy effective electron mass in InAs in comparison to InP and GaAs. Another effect that leads to exceed in velocity profile in InAs diode is due to larger electric field in the channel region [12-13] as it can be seen from Fig.5.

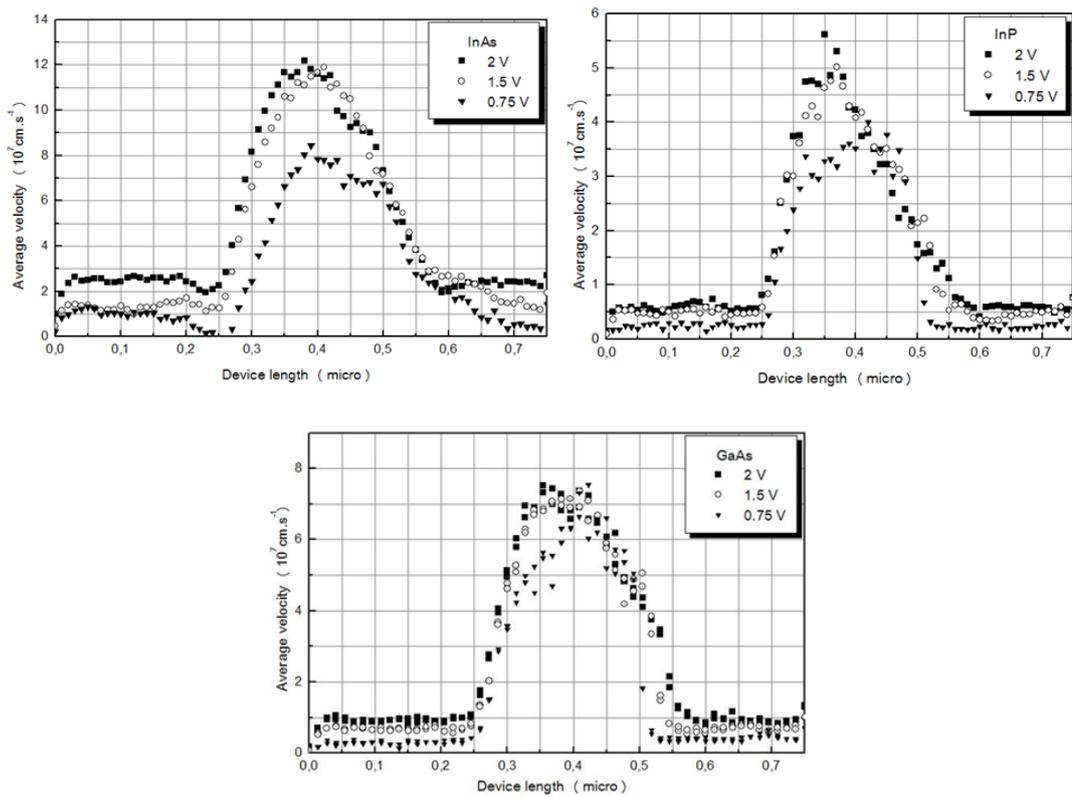


Figure 2: Comparison of the electron average velocity profile across a InAs , InP and GaAs $n^+ - i - n^+$ diodes for various anode voltages $V_A = 0,75V, 1,5V$ and $2V$, at $300K$

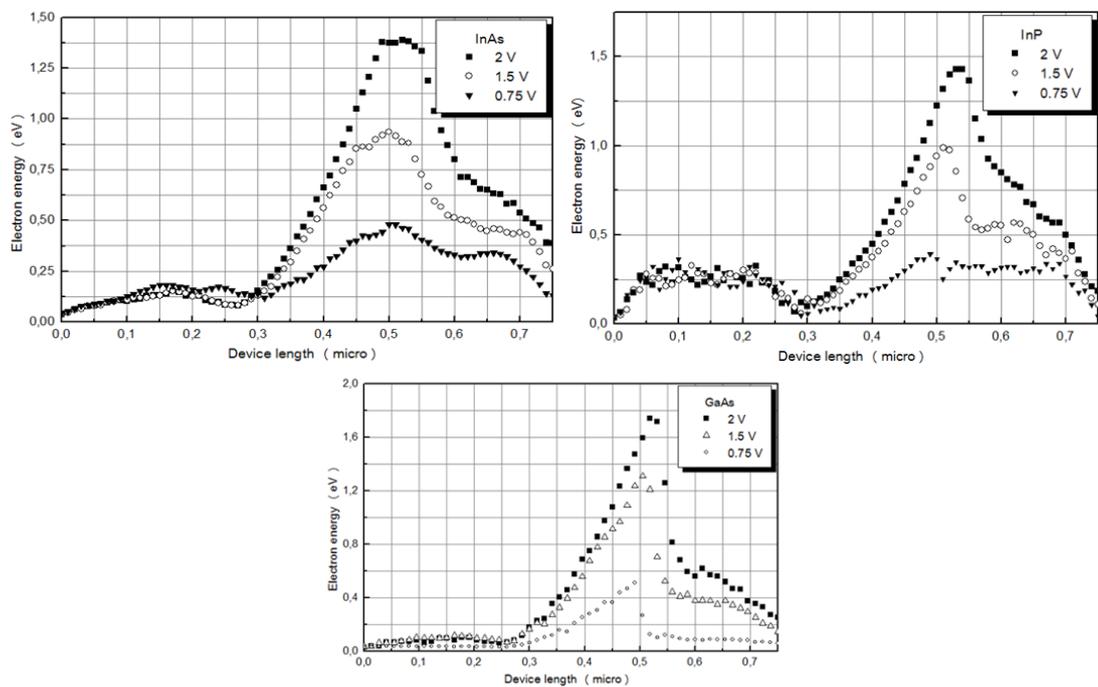


Figure 3: Electron energy distribution across a InAs, InP and GaAs $n^+ - i - n^+$ diodes, for various anode voltages $V_A = 0,75V, 1,5V$ and $2V$, at $300K$

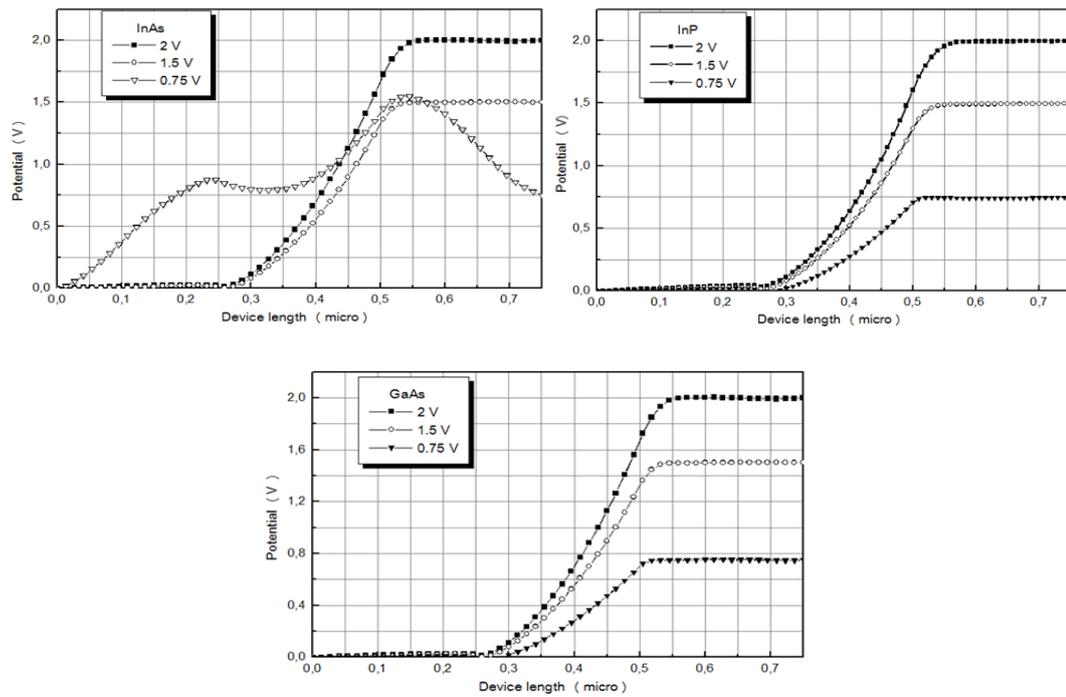


Figure 4: Distribution of the electrical potential in the InAs, InP and GaAs $n^+ - i - n^+$ diodes for various anode voltages $V_A = 0,75V, 1,5V$ and $2V$, at $300K$

Fig. 5 illustrates the electric field profile as function of device length in bias of $0,75V, 1,5V$ and $2V$ at $300K$ for InAs, InP and GaAs $n^+ - i - n^+$ diodes. This 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. Comparison of electric field variation in InAs, InP and GaAs diodes show that InAs-based devices should have higher output drain current since it depends on the electric field, and also exhibit velocity overshoot effects.

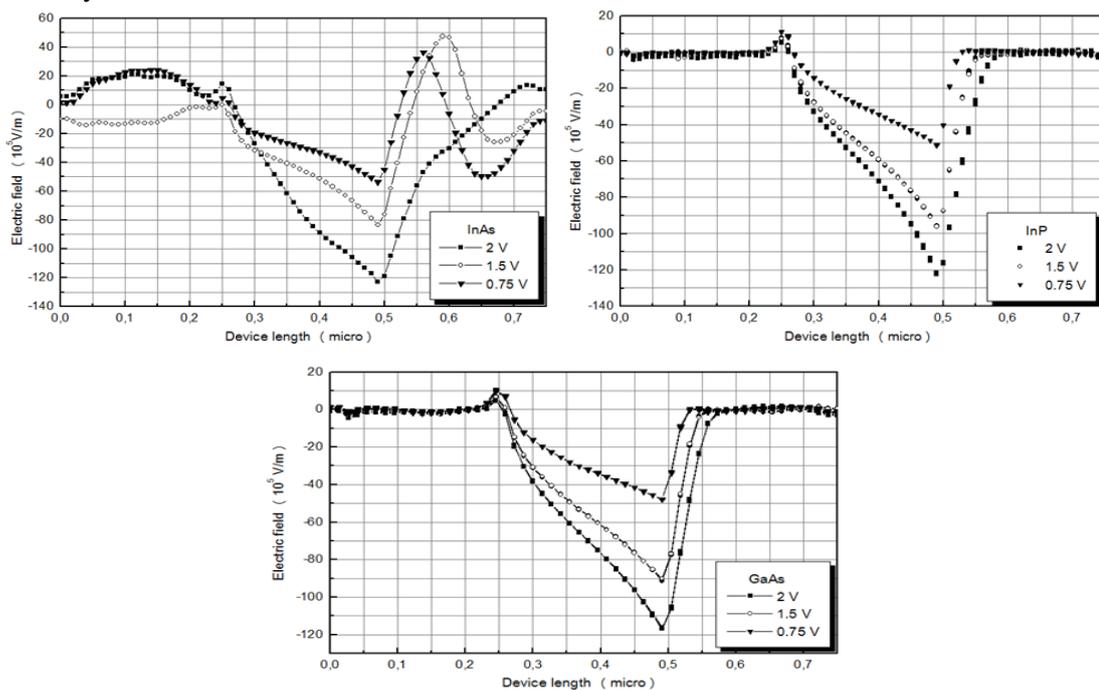


Figure 5: Electric field in the InAs, InP and GaAs $n^+ - i - n^+$ diodes for various anode voltages $V_A = 0,75V, 1,5V$ and $2V$, at $300K$

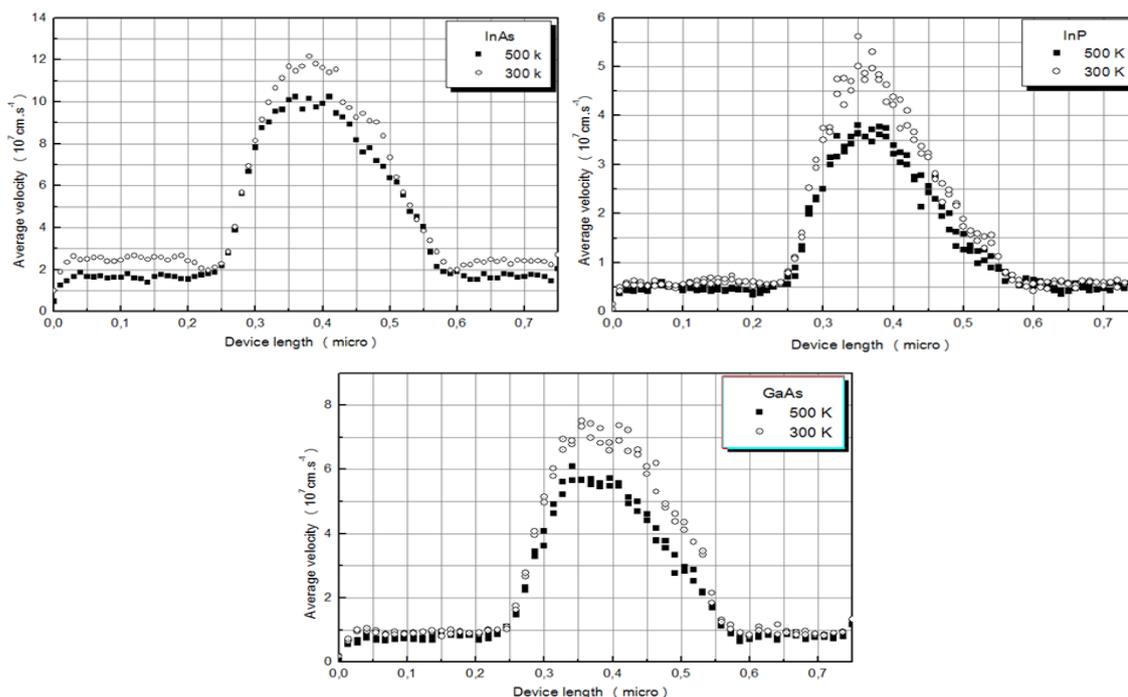


Figure 6: Comparison of the electron average velocity profile across the InAs , InP and GaAs n^+i-n^+ diodes, for $V_A=2V$ at different temperatures $T=300$ and $500K$.

Elevating the environmental temperature will result in higher scattering rates. Fig.6 compares the electrons average velocities across a diode with an active region length of $0,25 \mu\text{m}$ in bias of $V_A=2V$ at temperatures $T=300$ and 500 K . Raising the temperature to 500 K reduces the maximum drift velocity to a value of $11.10^7 \text{ cm.s}^{-1}$ in the case of InAs diode. This shows InAs characteristics are superior to InP and GaAs. Therefore, the InAs devices displayed substantially greater stability with respect to changes of voltage and temperature. This stability is mainly due to the ability of InAs to maintain a positive differential resistance at the drain contact due to ballistic effects under the gate. A similar decrease of drift velocity with temperature is seen in bulk material and is due to increased electron scattering.

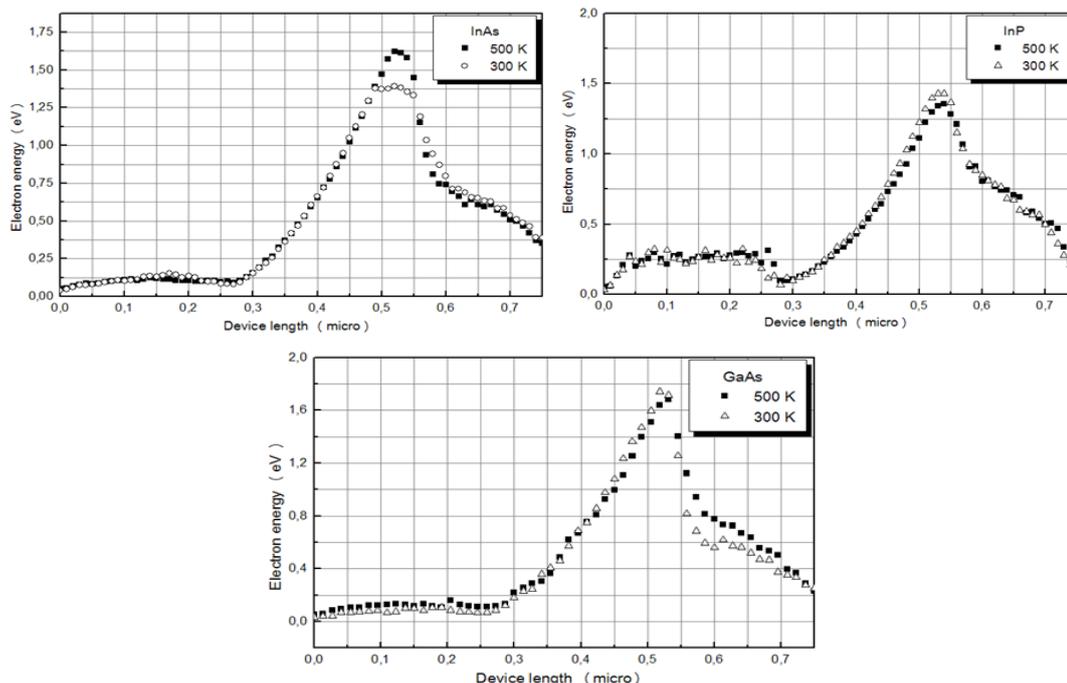


Figure 7: Comparison of the electron energy profile across the InAs , InP and GaAs n^+i-n^+ diodes, for $V_A=2V$ at different temperatures 300 K and $500K$.

It can be seen from Figs. 6 and 7 that increasing the temperature from 300 to 500 K causes some decrease in the electron transport characteristics of simulated diodes. As noted earlier, this effect is due to increased phonon scattering, which suppresses the heating of carriers by the electric field. Note, however, the effect is relatively small when considering the large increase in temperature.

Conclusion

In this paper, the results of simulations of electron transport in InAs, InP and GaAs n^+i-n^+ diodes have been reported. The anode voltages ranged from 0,75V, 1,5V to 2 V and lattice temperatures of 300K and 500K have been considered. The electrons injected from the cathode initially travel quasi-ballistically but there is substantial transfer to the upper satellite valleys as the anode is approached, resulting in a reduced average electron velocity in that region. 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. Raising the lattice temperature to 500 K reduces the peak drift velocity. Our results also show that InAs devices have better performance than InP and GaAs devices.

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