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Study of electron transport in N-type InAs substrate by Monte Carlo Simulation

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Résumé

Étude du transport d'électron dans le substrat InAs de type N par la simulation de Monte Carlo

La compréhension des phénomènes microélectroniques décrivant le comportement des porteurs dans les matériaux semi-conducteurs exige la connaissance de la fonction de distribution d'énergie; celle-ci étant obtenue par la résolution de l'équation de Boltzmann. Or, la solution analytique de l'équation de Boltzmann s'avère très difficile et très complexe. Actuellement plusieurs méthodes numériques sont employées avec succès pour résoudre cette équation, parmi lesquelles la méthode de Monte Carlo qui fait l'objet de ce travail.

La simulation par les méthodes de Monte Carlo est aujourd'hui un des outils les plus utilisés pour l'étude du fonctionnement physique des composants électroniques. Elle consiste à suivre l'évolution des paquets d'électrons dans l'espace réel, où chaque électron soumis au champ électrique dans le matériau entre en interaction avec le réseau cristallin. C'est un processus itératif composé d'une séquence de vols libres, entrecoupée d'interactions acoustiques, piézoélectriques, polaires et non polaires, inter-vallées, impuretés, ionisation et surface.

Nous avons appliqué cette méthode au matériau III-V dans le cas de l'InAs. Nous avons étudié le comportement des porteurs du point de vue dynamique et énergétique (variation de la vitesse et de l'énergie en fonction du champ électrique).

La simulation est appliquée, en tenant compte de la variation des porteurs en fonction du temps (mode non stationnaire), de l'effet de la température, et de l'effet de la concentration (dopage). Les résultats que nous avons obtenus s'avèrent comparables à ceux de la théorie.

Mots-clés: *Méthode de Monte Carlo, interactions, structure de bande, composants III-V.*

Abstract

The microelectronic comprehension of the phenomena which describes the behavior of the carriers in semiconductor materials requires the knowledge of energy distribution function. This distribution function is obtained by the resolution of Boltzmann equation which is very hard to solve analytically. Many methods based on modeling are actually successfully used to solve this equation. This Monte Carlo method is among of the most methods used for electronics components operations studies.

It consists to follow the evolution of electron packets in real space, where each electron subjected to the electric field present in material goes interact with the crystal lattice. It is therefore an iterative process made up from a whole coasting flights stopped by acoustics interactions, polar and non polar optics, piezoelectric, inter-valley, impurity, ionization and surface.

By applying this method to the III-V material, case of InAs, we have described the behavior of the carriers from dynamic and energetic point of view (speed and energy variation according to the field). The simulation is applied, taking into account variation of the carriers as a function of the time in the non stationary mode, the effect of temperature, and doping concentration. The results we obtained are demonstrated to be comparable to the ones of theory.

Keywords: *Monte Carlo method, interactions, structure of band, III-V components.*

1. Introduction

The knowledge of the electron energy distribution function is obtained from the resolution of the partial derivative Boltzmann equation; it makes possible to study the transport phenomena in semiconductor materials. Nevertheless, the analytical solution of this equation is very complex, often one calls upon the techniques of digital simulations. The simulation by Monte Carlo method is one of these techniques, makes it possible to accurately reproduce the various microscopic phenomena existing in semiconductors materials [1,2,3].

The results of simulation enable us to know the stationary and non stationary phenomena, and to get directly to important parameters in electronic dynamics such as speed and energy. The Monte Carlo method we employ to characterize the materials, uses a model with three valleys (Γ, L and X) [4], non parabolic. The Monte Carlo module includes electron scattering with polar optical phonons, inter- and intra-valley optical phonons, equivalent and nonequivalent inter-valley optical phonons, non-polar optical, piezoelectric, impurities, acoustic phonons, ionized and neutral impurity scattering. In addition, alloy scattering and strain effects [5] are considered for the InGaAs channel. All scattering rates are calculated with a form factor (the overlap integral) proposed by Matz [6,7].

In the present paper, we have studied arsenic of indium "InAs". It is therefore interesting in order to understand its operation to carry out a complete study of the characteristics of this material and to determine the influence of the external medium on the effects which it produces [8,9]. The simulation employed in our case makes it possible to follow the evolutions of representative particles in the various layers of materials as a function of the time.

2. The Monte Carlo method

The principle of this method consist in following the behavior of each electron submitted to an electric field $\vec{E}$, in real space and the waves vectors space [10-12], for that :

1 - We have associated for each carrier which we want to simulate the trajectory, an initial wave vector $\vec{k}_0$ and an initial vector position $\vec{r}_0$.

2 - We have used the procedure "self-scattering". It consists in building a distribution of time following a law whose expression is simplified by the introduction of a fictitious interaction to the null effects known as "self-scattering"[1]. The knowledge of the state of the electron is carried out during instant of time irregularly partitioned.

3 - With each of the time step we know, for each carrier, its wave vector $\vec{K}$ and that position $\vec{r}$ at the instant *t* where the measurement begins. Then for a carrier noted *"p"*, we know :

$$\vec{K}_p(t), \vec{r}_p(t), \vec{E}_p(t) = \vec{E}(\vec{K}_p) \qquad (1)$$

4 - We accomplish a coasting flight of duration Δt, so we will have:

$$\begin{cases} \vec{K}_p(t+\Delta t) = \vec{K}_p(t) + \dfrac{e\vec{E}}{\eta}\Delta t \\ \vec{E}_p(t+\Delta t) = \vec{E}(\vec{K}_p(t+\Delta t)) \\ \vec{r}_p(t+\Delta t) = \int \vec{v}_p(t)\,dt \end{cases} \qquad (2)$$

5 - We look for if there were an interaction during the interval of time Δt by pulling at the fate of a random number:

- If there were no interaction, the state of the carrier is not modified.
- If there were interaction, we place the interaction at the instant $t+\Delta t$ and one seeks $\vec{K'}_p$ after the shock by drawing lots from a random number, its state is defined now by [13,14] :

$$\begin{cases} \vec{K'}_p(t+\Delta t) \\ \vec{E}_p(t+\Delta t) = \vec{E}(\vec{K'}_p(t+\Delta t)) \\ \vec{r'}_p(t+\Delta t) = \vec{r}_p(t+\Delta t) \end{cases} \qquad (3)$$

3. Results and discussion

In order to show the interest in studying the phenomenon of electronic transport in InAs, we present a study in stationary and non-stationary mode.

3-1. Stationary mode

The directly accessible average sizes in simulation are speed and energy.
We present on *Figures 1 & 2*, the average drift speed and average energy as a function of electric field. It is noticed that around the critical field, the speed reaches its maximum value, and then it starts to decrease from (3.63 kV/cm).

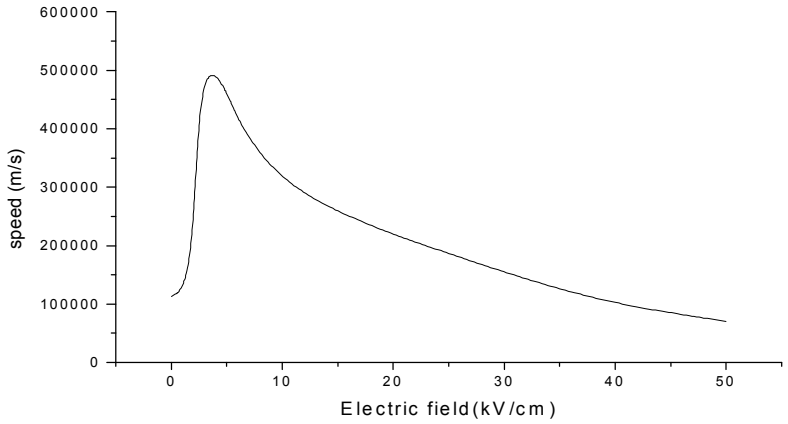

Figure 1 : *Speed profile according to the electric field E in InAs*

The carriers start to move from the valley Γ towards the higher valleys L and consequently their speeds fall (the carriers in the valley L are heavier than in the valley Γ).

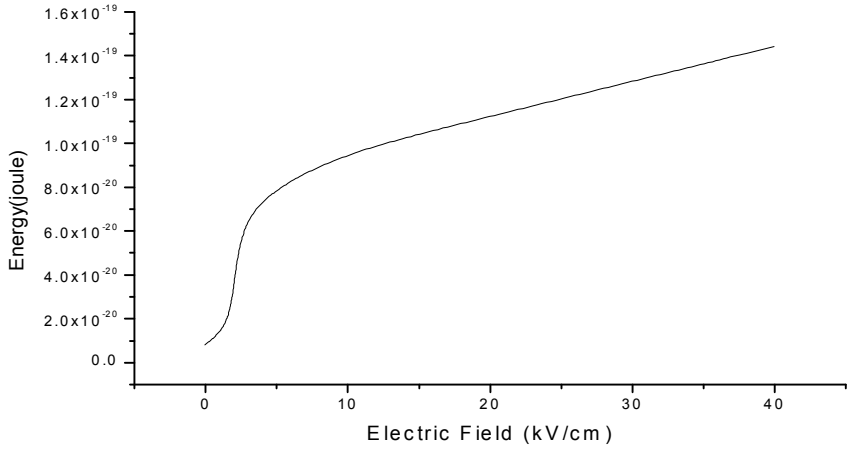

Figure 2 : *Evolution of energy over electric field E in InAs*

As soon as we apply a weak field the energy of the electrons is suddenly surplus compared to the new equilibrium conditions; thus, the electrons will transmit this energy during the interactions [1].

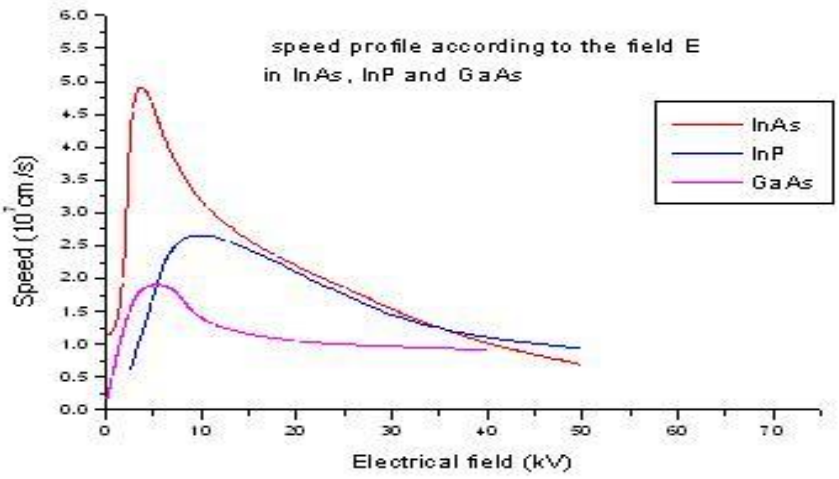

Figure 3 : *Speed profile* ε *according to the field E in InAs, InP and GaAs*

This energy will take ascending values but in an interval of the rather small values of field which varies from 0 kV/cm to 3.63 kV/cm. Once this value of field is exceeded, the carrier will have an energy which will have a linear variation according to the field.

If we make a comparison with other materials such as InP or GaAs, we can say that InAs has a slope $\frac{\Delta \varepsilon}{\Delta E}$ higher than those others materials *(Figure 3)*. In other words, we can say that in the same conditions, the carriers transport more energy than that transported in the cases of the two others materials.

This study shows that the materials which might present high over speeds are those for which both the mass is very low in central valley and a very high energy gap between the central valley and the most accessible side valleys, so that to allow the electrons to have enough time to acquire high speeds before being transferred.

Table 1 presents the ratio of effective masses (m^*_Γ/m_0) and the corresponding energy gaps (Δ_{Γ_L}) values respectively for InS, GaAs and InP compounds. These values show that we can expect better overspeed performances for InAs than that of GaAs and InP assuming the similar electrical field conditions.

Table 1 : *Ratio of effective masses (m_Γ^*/m_0) and the corresponding energy gaps ($\Delta_{\Gamma L}$).*

	InP	AsGa	InAs
m_Γ^*/m_0	0.08	0.063	0.022
$\Delta E_{\Gamma L}$	0.61 eV	0.33 eV	0.87 eV

Figure 4 shows the experimental results of the profile speed according the field E.

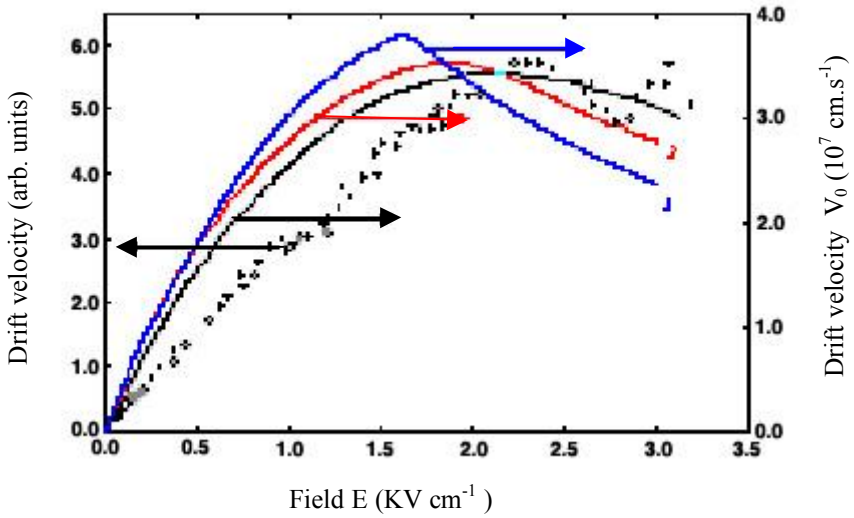

Figure 4 : *The experimental results of the profile speed versus the field E [15,16].*

3-2. Non-stationary mode

We notice "overspeed" phenomenon. The overspeed is a transient phenomenon in which electrons packets take values superior at the stationary mode speed *(Figure 5)*. For 10 kV/cm field, we observe absence of overspeed which implies absence of electron surplus. For 20 kV/cm field, the overspeed phenomenon is situated between 10^{-13} s and 10^{-12} s. And finally for 50 kV/cm field, the overspeed phenomena is situated between 10^{-13} s and 8.10^{-13} s.

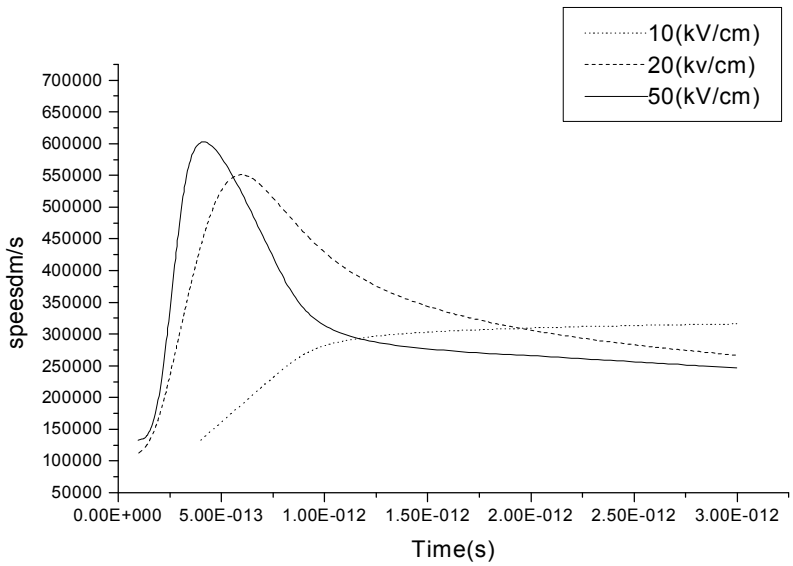

Figure 5 : *Evolution of speed versus time for various fields E*

Consequently we can conclude that there is a reduction in the maximum speed value with the reduction of the applied field. On the other hand when the field increases, the overspeed is shorter.

The role of the overspeed phenomenon is particularly concerned the determination of the performances in frequencies and power of the components carried out from studied material. It is conditioned by the latter, the transfer time of the electrons at a given distance. Therefore we have compared the possibilities offered by InAs regarding to other materials such as GaAs and InP. We have noted that the InAs material represents the phenomenon of overspeed better than those two materials.

3-3. Influence of doping

The effect of doping concentration on the carriers speed is determined by the application of a low field, this effect is illustrated in *Figure 6*. It shows the speed variation according to the field for various concentrations: 10^{16} cm^{-3}, 10^{14} cm^{-3} and an intrinsic semiconductor.

The curves are characterized by a reduction in the peak of speed and a small increase in the threshold field, consequently a reduction in mobility appears in low field.

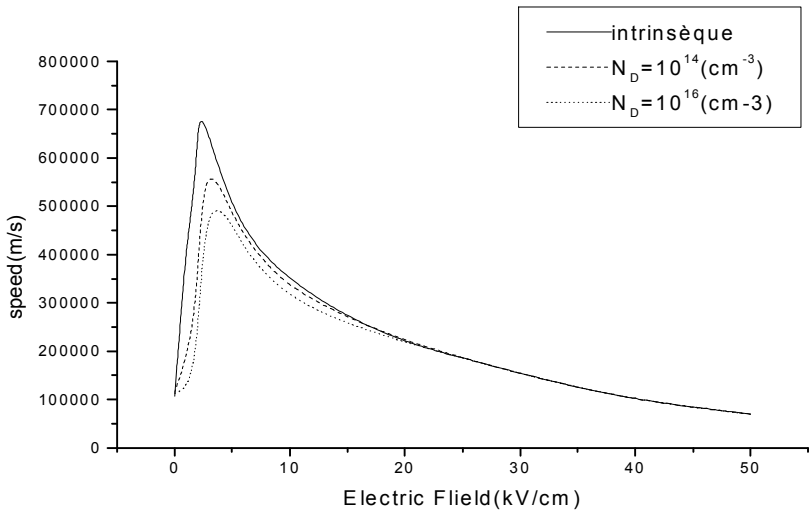

Figure 6 : *Speed profile according to the field E in InAs for different doping*

Therefore it is found that for an intrinsic semiconductor, the threshold field is equal to 2.31 kV/cm corresponding to a speed of 6.77×10^7 cm/s, for the concentration of 10^{16} cm^{-3} it is equal to 3.63 kV/cm for a speed of 4.92×10^7 cm/s, whereas for concentration of 10^{14} cm^{-3} the threshold field is equal to 3.13 kV/cm for a speed of 5.57×10^7 cm/s.

It is explained, the effect of doping is situated in a narrow interval of field and as soon as we begin to apply a strong field, the doping effect can be neglected because the curves converges [1].

3-4. Influence of temperature

We have follow the variation of speed according to the field for different temperature *(Figure 7)*, it is noted that for 300 K the maximum speed is equal to 5×10^7 cm/s for a threshold field of 3.87 kV/cm, whereas for 200 K the threshold field itself shell at 4.08 kV/cm and the speed itself decrease at 3.18×10^7 cm/s, as well as for 77 K the threshold field increases at 5 kV/cm which correspond at a maximum speed of 2.13×10^7 cm/s.

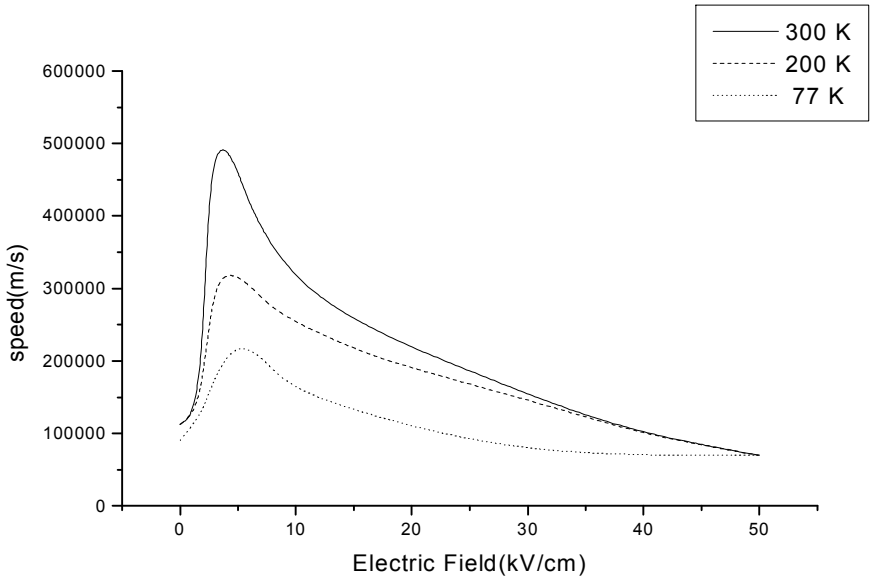

Figure 7 : S*peed profile according to the field E in InAs for different temperatures.*

We can conclude for that speed the temperature has an effect in low field [17]. Finally, the effect of the temperature is alternated for the high fields. It is noticed that the curves converges asymptotically starting from the time we reach high fields.

3-5. Influence of length

We have also studied the behavior of speed according to the field for various lengths of material *(Figure 8)*. The results show that at low field the material length practically does not have an effect on speed.

Once we get a field level above the threshold field, the speed decreases as the length of material is increased. This is due to the fact that when the length increases, the number of carriers also increases, consequently the number of interactions increases and therefore speed decreases.

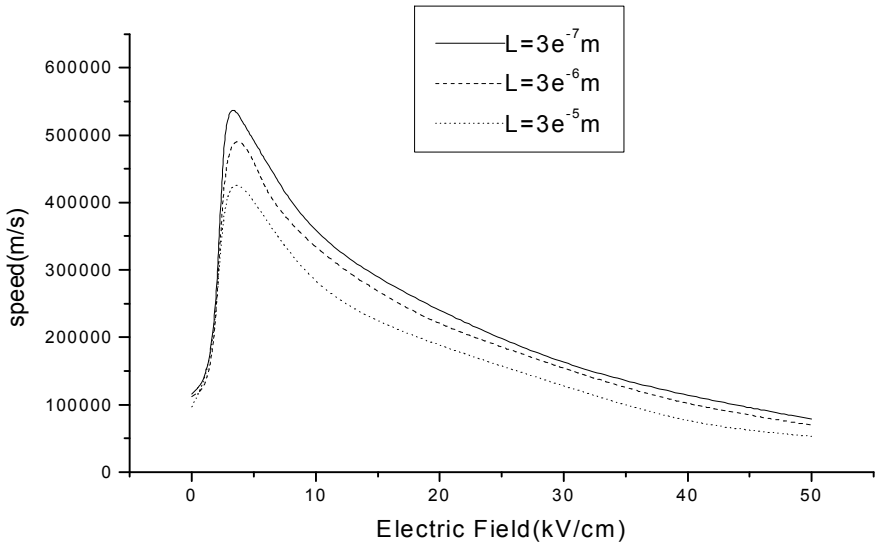

Figure 8 : *Speed profile according to the field E in InAs for various lengths of material*

Finally, when we are in conditions of extremely high field, the carrier has a speed not very alternative towards the change of length of material, because even in this condition, we have an asymptotic convergence of the curves.

4. Conclusion

We have presented the results obtained by the Monte Carlo method related to the semiconductor material InAs regarding to speed, energy, effect doping, the temperature and the length of material. The influence of these last three factors is predominant in the case of low field application.

These results are in agreement with the published experimental results, as well as the published numerical results. Simulation by Monte Carlo method constitutes an essential stage towards the knowledge of materials properties. Its flexibility in fact gives a tool adaptable to a great diversity of applications.

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