Steady State and Transient Study of The Electron Transport In N-Type GaSb Using Three Valley Monte Carlo Model

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Abstract

In this work, an investigation of the steady state and transient electron transport, at high electric field and high temperature, in n-type GaSb material was presented. We applied a Monte Carlo model considering the three valleys of the conduction band (Γ, L, X), isotropic and non-parabolic centered on the important symmetry point of the first Brillouin zone. This model provides a detailed description of the electronic dynamic and the electrons behavior at high electrical fields and high temperatures in these materials in each considered valleys. The calculation is made for different values of applied electrical field ranging from 50 to 600KV at different values of temperature. The scatterings rates taken into consideration are coulomb scattering acoustical and optical scattering, intra and inter-valleys scattering.

Keywords: *Gallium Antimonide, Electron Transport, Band Structure, Monte Carlo Method, Polar Scattering.*

1. Introduction

Over the last several years, the III-V binary compounds started showing considerable interest towards the study and use in microelectronic manufacturing [8, 19]. The Gallium Antimonide (GaSb) is one of these materials, with a direct bandgap that can be grown with high purity. The III–V ternaries and quaternaries (AlGaIn) (AsSb) lattice matched to GaSb seem to be the obvious choice and have turned out to be promising candidates for high speed electronic and long wavelength photonic devices [18].GaSb based structures are promising candidates for a variety of military and civil applications, notably for laser diodes with low threshold voltage, Photo-detectors, high frequency devices, and a promising material for optoelectronic semiconductor devices in the near infrared [4].

Because it's narrow bandgap (0.7ev), the GaSb-based structures are of great interest for application in mechanically stacked tandem solar cell, in thermo-photovoltaic [1] and in rechargeable lithium batteries [15]. As the unintentionally doped GaSb is invariably p-type in nature [14]. In our work we choose to study the n-type GaSb substrate. Recent investigations of the electron transport in the n-type GaSb are proposed in literature [4, 5, 16, 14]. In this work we investigate the steady state and transient electron transport properties, at high field and high temperature. It's known that the electron transport at high fields and high temperatures has reached an important stage in the last years and is dominated by the complex conduction-band structure well above the lowest band edge [8]. For the n-type GaSb the transport properties are more complicated due to the contributions from Γ, L and X conduction bands [18]. However, the electronic transport and phonons scattering is always described by models based on the resolution of the Boltzmann transport equation (BTE) who characterizes the modification of the function distribution of particles, caused by various actions, in space and time. The most used models are: the drift diffusion models, Hydro-dynamical models and Monte Carlo Models. This last is computationally intensive in fact that we can simulate the trajectory of a large number of electrons in physical and momentum space. Nowadays the microscopic transport model based on the Monte Carlo method appears to be adequate for studying of electronic transports characteristic in bulk and semiconductor devices [20]. In what follows, we give, in section 2, a detailed description of our MC code which uses analytic descriptions for both the electron bands and the phonon dispersion, and the results of transient and steady-state transport simulations are discussed in the last section.

2. Monte Carlo Model Description

Including the charges transport in semiconductors the Monte Carlo method is a statistical method, as a popular and effective mathematical tool for the study and analysis of the physical phenomena. This method was first applied to the study of transport by Kurosawa in 1966 [10] and is widely used since 1981 [11, 12]. The Monte Carlo method provides an additional advantage in which can be used as a theoretical laboratory in that parameters can be varied at will and their effects on observables assessed [17].
The principle of the method is to follow over time one or more electrons in real space and reciprocal space wave vector k. After the identification of symmetry L valleys which have minimum related lower to X valleys [11], this model has been used by many authors [6,8] and more recently by H. Arabshahi [16] in the studies of the electron transport in GaSb and other materials[17].Our model is developed considering the deformation potential of each considered valley, the effective masses, the dielectrics constant, the energy gap structures, and the main scattering mechanisms in details [3]. In general terms, the model is based on a process of drawing lots from the laws of probability associated with the electrons undergoing scatterings during their movements within the crystal lattice. The number of electrons simulated is 20000 electrons subjected to a varying field, at different temperature. Mainly, the simulation is done using the following steps [9, 7]: for each simulated electron "p" we associate an initial position "r", and an initial wave vector k, and using the method "individuals-dispersing" or "self-scattering", we introduce a fictitious scattering which aims to establish a time distribution.

$$\overrightarrow{K_p}(t), \overrightarrow{r_p}(t), \overrightarrow{E_p}(t) = \overrightarrow{E}(\overrightarrow{K_p}) \quad (1)$$

We performing free flight (no scattering) time period Δt constant, and low before the average time between two consecutive scatterings, such as:

$$\begin{cases} \overrightarrow{K_p}(t + \Delta t) = \overrightarrow{K_p}(t) + \dfrac{e\overrightarrow{E}}{\eta} \\ \overrightarrow{E_p}(t + \Delta t) = \overrightarrow{E_p}(\overrightarrow{K_p}(t + \Delta t)) \\ \overrightarrow{r_p}(t + \Delta t) = \int v_p(t)\,dt \end{cases} \quad (2)$$

During a free flight the electron is subject only to the electric field E, which changes the wave vector k according to the relationship [21]:

$$\frac{\partial \overrightarrow{K}}{\partial t} = \frac{q\overrightarrow{E}}{\hbar} \quad (3)$$

The integration of this equation, give the time evolution of the wave vector, and the knowledge of the band structure form $\varepsilon(\overrightarrow{K})$, permit to deduce the carrier's energy such as:

$$\varepsilon(1 + \alpha_i \varepsilon_i) = \gamma(k) = \frac{\hbar^2 k_i^2}{2m_i^*} \quad (4)$$

α_i denote the non-parabolicity coefficient of the valley "i". m_i^* is the relative effective masse in bottom of the valley. The density of state, by volume unity, associated to this model has the following form:

$$N(\varepsilon) = \frac{(2m_i^*)^{\frac{3}{2}} \cdot \sqrt{\varepsilon(1 + \alpha_i \varepsilon)}}{4\pi^2 \hbar^3}(1 + 2.\alpha_i \varepsilon) \quad (5)$$

The expressions of the energy and the density of state permits the formulation of the scattering probability that directly dependant to the energy. During the simulation, when scattering occurs, we place at time t + Δt, and we determine subsequently, its nature by lot, and we modify accordingly the energy and electron wave vector. Each process of scattering characterized by a density of probability S(k, k') characterizing the probability, for which an electron will pass from a state of energy K to another state K'[6].

$$\lambda_j(\vec{K}) = \int_{over\ .all\ .possible\ .states\ .K'.} S_j(\vec{K}, \vec{K}') \quad (6)$$

$$\lambda(K) = \frac{V}{8\pi^3}.2\pi \int_0^{\pi} \left[\int_0^{\infty} S(\vec{K}, \vec{K}') K'^2 .dK' \right] \sin\beta .d\beta \quad (7)$$

$\frac{V}{8\pi^3}$. denote the density of states in momentum space.

The factor 2π reflects the symmetry of revolution around all possible states. β represent the deviation angle. In Monte Carlo studies, the obtained results are strongly related to many physical parameters characterizing studied materials, which are sometimes badly known.

Therefore, the treatment of different information obtained, their analysis as function of the material parameters entered in the simulator, and compared to available experimental results, permit a real knowledge of physical effects and their consequences that occurs in the material. The basic and band structure parameters of GaSb material used in our simulation are shown in table1.

Table 1: Basic parameters of GaSb material [16, 18, 22]

Parameters	*Values*
Relative mass for gamma-valley	0.039
Relative mass for the L-valley	0.22
Relative mass for the X-valley	0.52
High-frequency permittivity	14.2
Low-frequency permittivity	15.5
Energies separation between gamma and L valley $\Delta_{\Gamma-L}$ [eV]	0.04
Energies separation between gamma and L valley $\Delta_{\Gamma-X}$ [eV]	0.33
Crystal density[g/cm^3]	5.613
Sound velocity [cm/s]	6070
Phonon energy (mev)	29

3. Results and Discussions

The Monte Carlo model adopted in this work is used for calculating and retrieval features of electronic transport in the n-type GaSb in the transitional regime. Interestingly, before describing the results and interpret them, establish a function of electric field and the valley occupied a hierarchy between the different scatterings experienced by the user. The results achieved by this model are given in the figures below. In '*Γ*' Valley, if the electron energy is very weak, then the scatterings predominate with a fairly low probability. According to Figure 1, the predominant scatterings for electrons in the valley *X* and L are those with polar optical phonons, with low wave vector. These scatterings are accompanied by an absorption or emission of a phonon. In this case the electron energy varies by an amount equal to the phonon energy $\hbar w$.

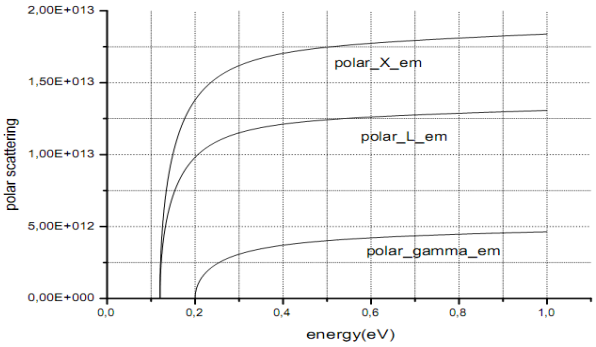

Fig. 1 Polar emission scattering rate

When the electron energy is sufficient, the emission of a phonon is a much more likely that absorption. The beginning of the phonon emission is easily identified in the curve of the valley from 40 mev. Also, the scatterings probabilities are greater in emission than that for absorption, and their value increases significantly when the electron energy increases.

Because of the dispersion relation of phonons is not constant; in this case the scatterings rate remains more complicated to calculate, and they occur when the ions through the crystal vibrate in the same direction.

According to Figure 2, due to the high value of effective mass, these scatterings are important in the X valley and increase more and more as energy increases. For high enough fields, the acoustic scatterings become dominant and subsequently the electron energy will be important. But as soon as the electron acquired energy greater than the energy separation $\Delta_{\Gamma L}$ and $\Delta_{\Gamma X}$ the transfer to the L and X valley become possible.

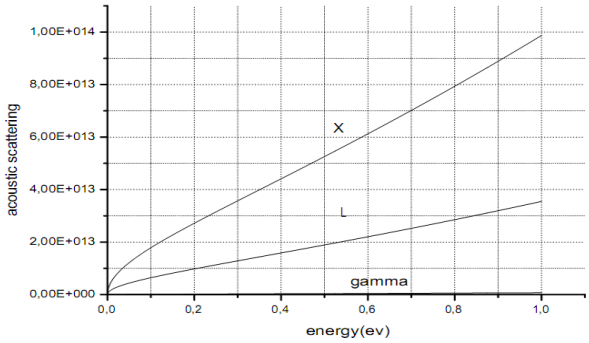

Fig. 2 Acoustic scattering rate .

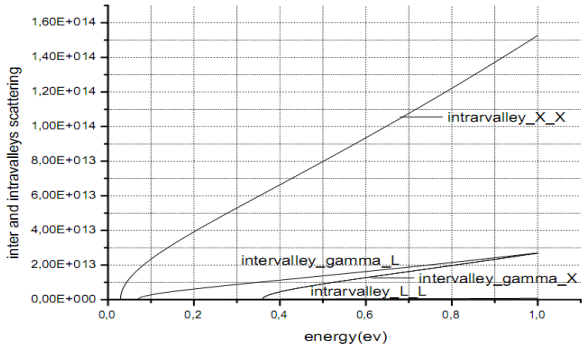

Fig. 3Piezoelectric inter and intra-valley scattering rate

Thus, when energy increases, we can see the beginning of the other type of scattering inter and intra- valley (figure 3). We can say that from energy for which transfers to the L and X valleys are possible, these processes are predominant. Piezoelectric interaction types are resilient and they are important in low field especially after the first transfers to valley level. Its main effect is decrease the value of mobility at low field. For acoustic interactions are the most favored among the elastic scatterings, they are mainly caused by the electron doping effects.

The figure below give the electronic population as a function of time in each considered valley gamma, X and L for an applied electric field of 400KV/cm. This result shows that the inclusion of the satellite valleys in the simulation is very important [16]. When the applied field is significant and exceeds the threshold value, the inter-valley scattering becomes important into the satellite valleys L and X. This can be explained by the fact that electrons closed to the valley minimum have small kinetic energies, then more scattered. Thus, due to the combined effect of a lower gamma effective mass (0.039), lower separation energy ($\Delta_{\Gamma-L}$ and $\Delta_{\Gamma-X}$), and the lightly lowers phonon scattering rate within the central valley gamma, the intervalley scattering is substantially larger in GaSb over the range of applied electric fields.

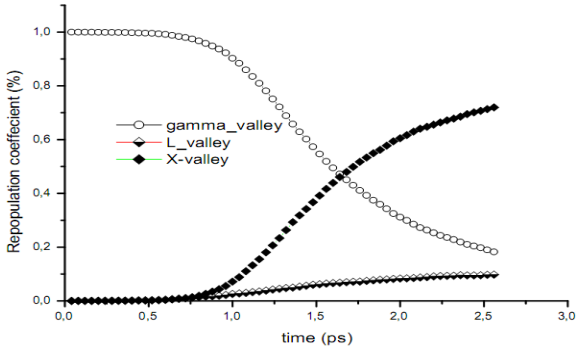

Fig. 4 The electronic population of the valleys depending on the time

The evolution of the electron drifts velocity as a function of field at room temperature was studied (see figure 5). There is a pronounced peak drift velocity located to $25x10^6$cm / s that occurs at a significantly lower electric field [16]. This result is the same obtained by H. Arabshahi [16]. In Central Valley Γ, the electrons have small effective masses (0.039 m_0), as soon as one applies a lower energy than the phonon scatterings there are only at the Γ valley.

By increasing the applied field, speed increases and reaches its maximum value near the threshold field (~1KV/cm), at which time the electron energy will be higher than the phonon, we have in this case a transition to the holder's side valleys L and X. When increasing the electric field, the speed decreases because the electrons are heavier side valleys. The interactions involved in this case the interactions are polar optical, intra and intervalley interactions.

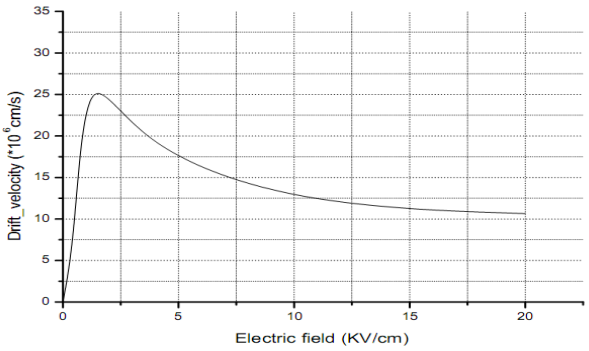

Fig. 5 Electron drifts velocity in GaSb bulk

When the electrons are subjected to fields largely varying in time (non-stationary mode), a phenomenon of overshoot velocity appears. This phenomenon was often studied by many authors, which did not fail to underline the practical interest of this phenomenon, in particular on the level of the submicronic components. Figure 6 give the look of the average electrons velocity. The calculation is made for electric fields ranging from 50 to 600KV/cm. We note a notable maximum velocity for the strong fields. Due to the low effective mass in valley, this maximum is important at high field ($9.5x10^7$ cm/s for a value of 600KV/cm of the electric field and a donor concentration of 8.10^{17} cm^{-3}). The maximum velocity is situated between 0.5 and 4 ps. More energy relaxation becomes effective as the distribution function and the drift velocity decreases.

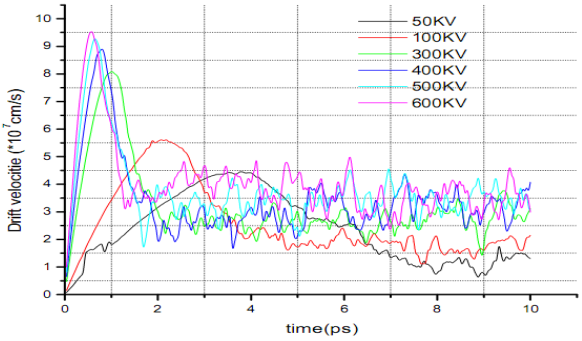

Fig. 6 Electron drifts velocity in GaSb bulk at 300K for different value of the applied electrical field

The temperature effect on the electrons velocity is also studied. The relating curves to drifts velocity at different values of temperature, for an electric field of 400KV/cm are presented.

When the temperature increases the peak of velocity decreased. This last is due to the effect of acoustic scattering that becomes important as temperature increases and to the increase in the lattice vibrations (result of the increase in the temperature) supporting thereafter the transitions inter-valley and intra-valleys in another side. Nevertheless, the electron saturation velocity is significant in the GaSb what explains the increasing interest of this material within the industrial framework. Thereafter, polar optical interactions become dominant among all elastic scatterings.

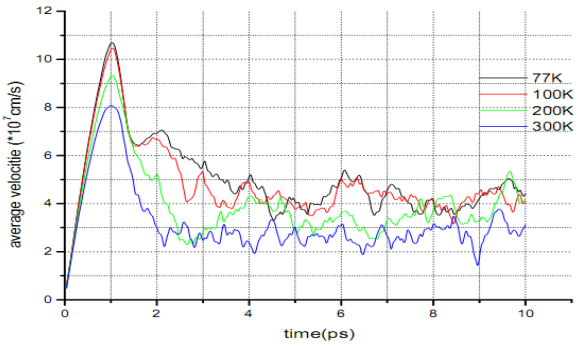

Fig. 7 Electron drifts velocity in GaSb bulk at different values of the temperature for an applied electrical field of 300KV

4. Conclusion

The electron transport in the n-type GaSb was studied. We adapted the Monte Carlo model written in FORTRAN, which is accurate, reliable and sometimes even simpler than the conventional numerical techniques. The transport characteristics and properties of GaSb obtained by this model, are satisfactory compared to other calculations in literature, and inform us about electronic dynamics as well as the behavior electric high fields and high temperatures in this material. The obtained results show that GaSb have a peak velocity little weak compared to other material. Therefore, we note an important overshoot velocity at low temperature (~11*10^7cm/s at 77K). The overshoot velocity phenomenon is major, particularly, in the determination of executions in the frequency and power components made from the material studied. However, analysis of results as the drift velocity of electrons demonstrates the remarkable effect of temperature and applied field on the dynamics of holders within the lattice as a result of interaction mechanisms.

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