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Semi classical three-valley Monte Carlo simulation analysis of steady-state and transient electron transport within bulk $Ga_{0.38}In_{0.62}P$

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Abstract—to simulate the phenomenon of electronic transport in semiconductors, we try to adapt a numerical method, often and most frequently it's that of Monte Carlo. In our work, we applied this method in the case of a ternary alloy semiconductor GaInP in its cubic form; The Calculations are made using a non-parabolic effective-mass energy band model. We consider a band of conduction to three valleys (ΓLX), major of the scattering mechanisms are taken into account in this modeling, as the interactions with the acoustic phonons (elastic collisions) and optics (inelastic collisions). The polar optical phonons cause anisotropic collisions, intra-valleys, very probable in the III-V semiconductors. Other optical phonons, no polar, allow transitions inter-valleys. Initially, we present the full results obtained by the simulation of Monte Carlo in GaInP in stationary regime. We consider thereafter the effects related to the application of an electric field varying according to time, we thus study the transient phenomenon which make their appearance in ternary material

Keywords—Monte Carlo simulation, steady-state electron transport, transient electron transport, alloy scattering.

I. Introduction

THE carrier transport modeling of GaInP and InP materials has only recently begun to receive sustained attention, now that the progress in compounds and alloys has resulted in the production of valuable materials for the electronics industry. Nowadays the microscopic Model of transport based on the Monte Carlo method seems to be effective and adequate to study the characteristics of electronic transport in materials and devices semiconductors. In this work we treat the electron transport of material GaInP which can be used in the design and the analysis of performance of the electronic devices in various conditions [1]–[3].

To thus study these components of very small dimensions, many formalisms were proposed. Among the microscopic models most complete, are reproduced the simulations based on the Monte Carlo methods which remain a reference, on which one rests to develop empirical models of mobility. In the domain of electronics, these simulations make it possible to study not only the properties of transport finely, but also a great Number of physical phenomenons. The results obtained by simulation are confronted, permanently with the experimental data of the literature [4]–[7], in order to discuss the assumptions and the relevance of the ideal model. In this communication, we present Monte Carlo calculation of the transport conditions of the electrons in stationary regime and no stationary (transient) regime in InP, and GaInP. We show the effect of the electric field on the transport of electron in transient state. The differences in the properties of transport are analyzed in terms of significant material parameters [8].

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II. Model details

In order to calculate the drift velocity of electron for high electric fields, the consideration of the satellite valleys of the bands of conduction is necessary. One of the essential entries of the model is the structure of energy band. The first principle of the structure of band of InP and GaInP envisages a direct gap of band located at the point Γ and lower satellite valleys of band of conduction of energy as in point X and L. In our simulation Monte Carlo, the valley of Γ, the three equivalent valleys of X, and the four equivalent valleys L were represented by spherical, no parabolic and analytical expressions of mass effective of the following form

$$E(k)\left[1+\alpha_i\,E(k)\right]=\frac{\hbar^2}{2}\left[\frac{k_x^2+k_y^2}{m_\perp^*}+\frac{k_z^2}{m_\parallel^*}\right] \qquad (1)$$

Where,$m_\perp^*$ and $m_\parallel^*$ are the transverse and longitudinal effective masses at the band edge and α_i is the non-parabolicity coefficient of i-th valley.

The material parameters of interest for use in an ensemble Monte Carlo simulation are presented in Table I for bulk $Ga_{0.38}In_{0.62}P$ [9]–[11]. These parameters were obtained either directly.

From the literature, from a k^* calculation of the band structures of this material, or in many cases from suitable interpolations of the parameters for the constituent binary compounds, InP, and GaP. The form factors used in calculating the band structures were derived by interpolating the form factors for the constituent binary compounds [12].

III. Calculated results

Fig.1 shows the characteristic speed-field out of InP material and $Ga_{0.38}In_{0.62}P$ at ambient temperature and with a

TABLE I
MATERIAL PARAMETERS FOR $Ga_{0.38}In_{0.62}P$

Parameter	Value and units
Optical phonon energy (eV)	0.0464[b]
Density	4.47 g/cm^3[b]
Dielectric constants:	
Low frequency,ε_0	11.75[a]
High frequency,ε_∞	9.34[b]
Energy gap	1.92 eV[a]
Effective mass:	
Γ valley	0.105[a]
L valley	0.242[a]
X valley	0.61[a]
Heavy hole	0.48[a]
Light hole	0.14[a]
Split off-hole	0.226[a]
Valley separation energies:	
$\Delta_\Gamma L$	0.125 eV
$\Delta_\Gamma X$	0.125 eV
Sound velocity	4.33×10^5 cm/s[b]
$\bar{u} = \sqrt{1/3u_e^2 + 2/3u_t^2}$	
Longitudinal	5.49×10^5cm/s[b]
Transverse	3.62×10^5cm/s[b]
Split off-hole	0.105 eV[a]
Def. potential constants:	
a	7.82[b]
b	1.90[b]
d	4.75[b]

[b] [8], [7] [a]

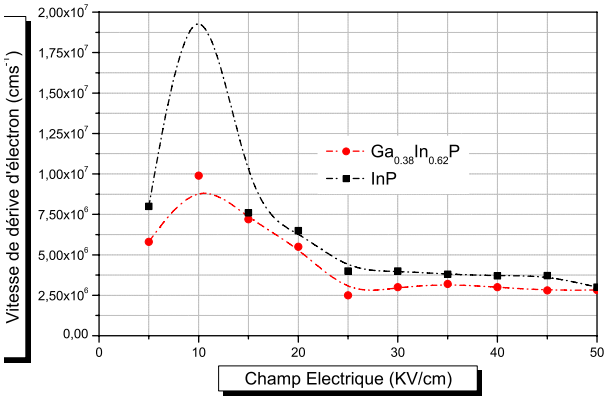

Fig. 1. Calculated steady-state electron drift velocity in bulk Zinc-blende InP, $Ga_{0.38}In_{0.62}P$ at room temperature with a background doping concentration of 1016 cm^{-3}.

concentration of doping of 10^{16} cm^{-3} and with an electric field applied to one of the cubic axes. As you can observe it, the characteristic of speed-field shows a peak for InP and $Ga_{0.5}In_{0.5}P$ with approximately 2×10^7 $cm \cdot s^{-1}$ and 0.9×10^7 $cm \cdot s^{-1}$ respectively. The curve speed-field typically presents a reduction the speed of electron, when the electric field increases above the value threshold. This effect is due to the transfer of the electrons starting from the central valley Γ with a state of low energy and a mobility high to a higher valley with the state of high energy and of a low mobility.

The average energy of electron according to electric field applied is depicted in Fig.2. It's clear that initially the curve of energy shows a high monotonous increase with the increase in

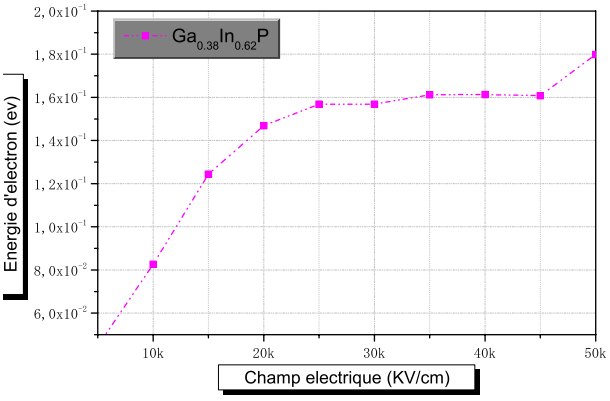

Fig. 2. Average electron kinetic energy as a function of applied electric field in bulk $Ga_{0.38}In_{0.62}P$ using the non-parabolic band Model at different temperatures.

the external field. Then, the increase in energy becomes slow beyond a certain value of electric field which corresponds to the breaking value. This characteristic is a consequence of the transfer of electron starting from the valley Γ to the valleys L and X the rise initially of energy is due to the dominant contribution of the acoustic mechanism of diffusion until it reaches with a certain threshold value approximately about 10 kV/cm. Beyond this value, the optical mechanisms of diffusion rather play an energetic role than acoustic. Since this process is inelastic, the curve energy of electron has a significant variation on its slope; indeed it does not increase also fast as it increases in the initial fields.

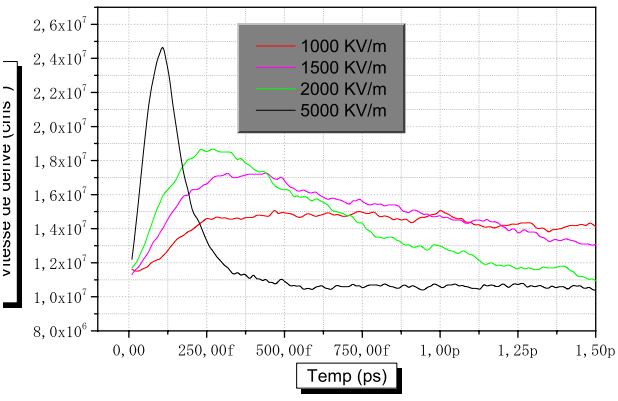

Fig. 3. A comparison of the velocity overshoots effect exhibited by $Ga_{0.38}In_{0.62}P$ semiconductor as calculated by Monte Carlo simulation. The donor concentration is 10^{17} cm^{-3} and the temperature is 300 K.

To highlight the effects of no stationary transport which can appear in ternary Materials, and more precisely in alloy $Ga_{0.38}In_{0.62}P$, we examined the behavior of the electrons subjected to variations abrupt of the electric field of variable nature. The response in transient state of its electrons and in this alloy is exhibit in the Fig.3.

The overshoot velocity initially increases more quickly with the electric increase in field by reason of the low effective mass of the valley Γ. For an electric field lower than the critical field ($\inf 10kV/cm$), the effect of overshoot is very that little or is not completely observable in the GaInP alloy. From 15 kV/cm up to 50 kV/cm, the velocity starts to present a peak. This peak, for the field 15 kV/cm, is of $1.7 \times 10^7\ cm \cdot s^{-1}$ for a time of 315 fs. For the field 50 kV/cm, maximum speed is of $2.45 \times 10^7\ cm \cdot s^{-1}$ for a time of 108 fs.

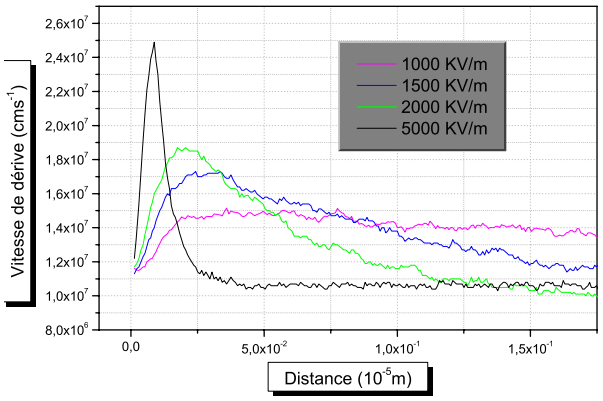

Fig. 4. A comparison of the average electron velocity as a function of the displacement for various applied fields in semiconductor $Ga_{0.38}In_{0.62}P$.

Fig.4 illustrates the average velocity of the electrons in GaInP according to the distance. We note that, for the field applied of 10 to 50 kV/cm, the average velocity of the electrons reaches the stable state quickly with little or no overshoot velocity. It's suggested that in GaInP, 10 kV/cm is the critical field for the appearance of overshoot velocity. As mentioned below, 10 kV/cm also corresponds to the peak in the characteristic of speed-field.

On the other hand it's clear that for an electric field of 50 kV/cm, the speed reached $2.45 \times 10^7\ cm \cdot s^{-1}$ after 108 fs with 67 nm distance traveled.

IV. Conclusion

The Monte Carlo methods allowed by the simple observation of a whole of electrons during time, to highlight the most significant characteristics of the properties of GaInP in stationary regime and transitory.

Using valley models to describe the electronic band structure, curve velocity-field characteristics are in fair agreement with other schedule. Saturation drift velocities $2.7 \times 10^4 ms^{-1}$ match recent measurements on low-doped bulk Samples. On the other hand calculated velocity-field characteristics show that the inter-valley Transitions in high electric fields play an important role in GaInP, despite a large Separation between the central and upper valleys.

The inter-valley transitions lead to a large negative differential conductance. It should be noted that the results exhibited above depend mainly on the exactitude of the reported parameters. While waiting for other works of experimental, this article is used as preliminary stage towards the comprehension of the properties of transport and the potential of device materials of GaInP.

Research is thus far from being finished, they are always in advance for any knowledge on these materials especially in the field of optoelectronics. This simulation method is used by several researchers who made to him improvements by increasing the number of particles studied, for example, to make it more accurate.

References

[1] S.-L. Fu, T. P. Chin, M. C. Ho, C. W. Tu, and P. M. Asbeck "Impact ionization coefficients in (100) GaInP", American Institute of Physics, 1995.
[2] U. V. Bhapkar and M. S. Shur, "Ensemble Monte Carlo study of electron transport in wurtzite InN", J. Appl. Phys., 1997, 82, 1649-1654.
[3] H. Arabshahi, M. R. Khalvati, and M. Rezaee "Temperature and Doping Dependencies of Electron Mobility in InAs, AlAs and AlGaAs at High Electric Field Application" Brazilian Journal of Physics, September, 2008
[4] H. Arabshahi, Modern Physics Letters B. 21, 199 (2007).
[5] C. Moglestue, Monte Carlo Simulation of Semiconductor Devices 1993 pub. Chapman and Hall.
[6] M. Allali, C. B. Sorensen, E. Veje, and P. Tidemand-Petersson, Phys. Rev. B 48, 4398 (1993).
[7] D. C. Cameron, L. D. Irving and C. R. Whitehouse, "Hot carrier relaxation in InP and GaAs", Thin Solid Films., 1983, 103, 61-66.
[8] B. E. Foutz, L. F. Eastman, U. V. Bhapkar and M. Shur, "Full band Monte Carlo simulation of zincblende GaN MESFET?s including realistic impact ionization rates", Appl. Phys. Lett.,1997, 70, 2849-2854
[9] M. Levinshtein, S. Rumyantsev "Handbook Series on Semiconductor Parameters" Volume 2 Ternary and Quaternary III-V Compounds
[10] E. O. Kane, "Band structure calculation in group III and IV materials", J. Phys. Chem. Solids, 1957, 1, 249-253
[11] A. Hamdoune, B. Bouazza, A. Guen-Bouazza, A. Lallam et N. Chabane-Sari "Développement de la mthode de Monte Carlo pour le calcul des interactions et du transport lectrique dans les semi-conducteurs ternaires" Afrique Science (2007).
[12] C. Sayah, B. Bouazza, A. G. Bouazza et N. Chabane-Sari "Etude théorique du transport électronique par la simulation Monte Carlo dans le quaternaire $In_{0.863}Ga_{0.137}As_{0.3}P_{0.7}$" Afrique SCIENCE 04(2) (2008) 186–198 ISSN 1813-5.