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Study of the Phenomena of Transport in the $Hg_{0.8}Cd_{0.2}Te$ Substrate of n-type by the Monte Carlo Method

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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. The Monte Carlo method is among the most methods used for studying electronics components operations.

It consist 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 optical polar interactions, and, impurities, ionization and Disorder of alloy. By applying this method to material $Hg_{0.8}Cd_{0.2}Te$ 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 similar to the theory. *Copyright © 2012 IFSA.*

Keywords: Simulation, Method Monte Carlo, Semi-conductor on base $Hg_{0.8}Cd_{0.2}Te$, Electric field

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1. Introduction

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. The Monte

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By applying this method to material $Hg_{0.8}Cd_{0.2}Te$ 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 similar to the theory. Knowing the distribution function of energy is obtained from solving partial differential equation of Boltzmann, and it is possible to study transport phenomena in semiconductor materials. Nevertheless, the analytical solution of this equation is very complex; it often relies on techniques of numerical simulations.

The simulation by the Monte Carlo is one of these techniques; it allows reproducing exactly the various microscopic phenomena existing in semiconductor materials [1-3]. The simulation results allow us to know the stationary and no stationary phenomena, and to obtain directly the important parameters in the dynamic electronics such as speed and energy. The $Hg_{1-x}Cd_xTe$ is a material used in the field of infrared detection camera. The composition x = 0.2, which we focus, allows a photo detector in the window 8-12 microns at a temperature of 77 K. Under these conditions, the material in a gap of around 100 meV in addition, it has a high electron mobility and electron transport system is in hot carrier for electric field values relatively low[2].

In this work, we present a Monte Carlo simulator only for electrons. The contribution of holes is in fact neglected because of their effective mass of about a hundred times greater than that of electrons. Energies in the valleys L and X is large compared to the band gap, band structure simulated is reduced to the Γ valley alone Fig. 1 considered non-parabolic.

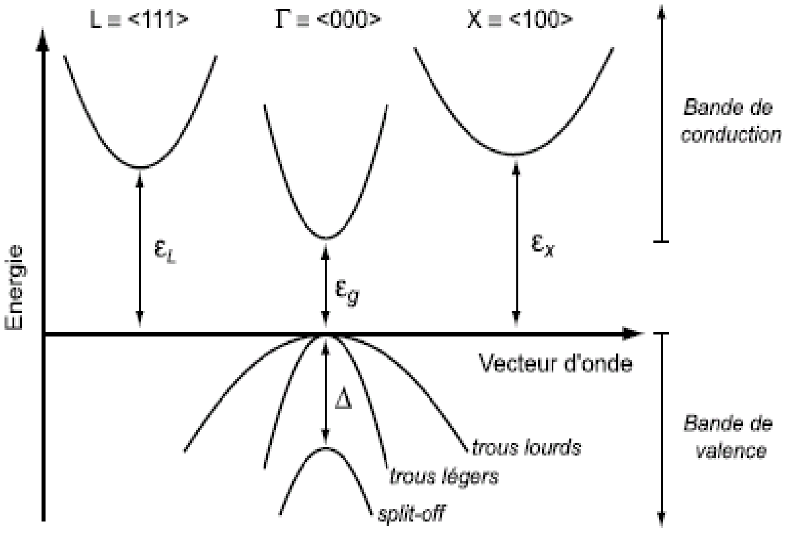

Fig. 1. Model for the band structure of a semiconductor.

Crystallizing in the $Hg_{1-x}Cd_xTe$ blended structure.

The collision processes considered are collisions with ionized impurities, two polar optical phonon modes and the alloy disorder. Depending on the study to be undertaken, we can choose whether to introduce a process of ionizing collision, and the phenomenon of electron multiplication.

The simulation used in our case allows monitoring changes in particle representation in various layers of materials with time.

2. Monte Carlo Method

The simulation by the Monte Carlo is now one of the most widely used techniques for the study of physical functioning electronic components and offers the ability to reproduce faithfully the microscopic phenomena occurring in the sensitive semiconductor materials [4].

The general idea of the Monte Carlo Simulation (MCS) in modern simulators is to study the dynamics of charge carriers during their displacement in the semiconductor materials.

This movement generally comprises two stages:

- The movement under the influence of external forces, that is to say free range, and
- Reaction to the wearer's physical interactions in the material, or diffusion (scattering) [5].

The principle of this method lies in the behavior of individual electrons subjected to an electric field in real space and the space of wave vectors for the:

1) We associate to each holder that we will simulate the trajectory, an initial wave vector k0 and an initial vector position.
2) We used the proceeds "self-dispersing". It is establishing a distribution of time according to a law whose expression is simplified by introducing an interaction dummy for null effects known as "self-dispersing" [2]. Knowledge of the state of the electron is made during the instant of time divided irregularly.
3) At each step we know, each carrier wave and its vector position at time t or the measurement begins. So for a "p» remarkable by hand we know that:

$$K\,p\,(t),\ r\,p\,(t),\ E\,p\,(t)= E\,(K\,p) \tag{1}$$

4) We do accomplish a flight (gliding) of the timeΔ t, so we have:

$$\begin{cases} K_p(t+\Delta t) = K_p(t) + \dfrac{eE}{m^*}\Delta t \\ E_p(t+\Delta t) = E(K_p(t+\Delta t)) \\ r_p(t+\Delta t) = \displaystyle\int V_p(t)dt \end{cases} \tag{2}$$

5) We are looking if there was an interaction during the time interval ΔT by pulling at the fate of a random number:

- If there is no interaction, the status of the wearer is not modified.
- If there was interaction, we place the interaction at time t+Δt and seek for$\overrightarrow{K_p}$) after the shock spells by drawing a random number, its state is now defined by [5.6]

$$\begin{cases} K_p(t+\Delta t) \\ E_p(t+\Delta t) = E(K_p(t+\Delta t)) \\ r_p(t+\Delta t) = r_p\ (t+\Delta t) \end{cases} \quad (3)$$

3. Results and Discussion

To show interest in studying the phenomenon of electron transport In $Hg_{0.8}Cd_{0.2}Te$, we present a study in stationary and mobile.

3.1. Stationary Mode

The average sizes directly accessible in the simulation are the speed and energy.

See Fig. 2 and Fig. 3, we have plotted in Fig. 2 the velocity versus electric Field. At low electric fields (below 50 V/cm) Fig. 2, the velocity increases linearly with the field, the probability of occupation of states of high energy is very low. Thus, electronic transitions are essentially due to ionized impurities and that for a value of electric field, the speed is even lower than the density of ionized impurities is important.

Note also that for an electric field of 500 V/cm, the velocity in the $\mathbf{Hg_{0.8}Cd_{0.2}Te}$ remains high, since it is of the order of 4 × 10^5 m/s.

This energy takes increasing values but in a rather small range of values of the field changes from 0 (kV/cm) 5 (V/cm) for which the average energy remains almost constant. In this case, the different collisions are sufficient to dissipate the energy it transmits to the free electrons.

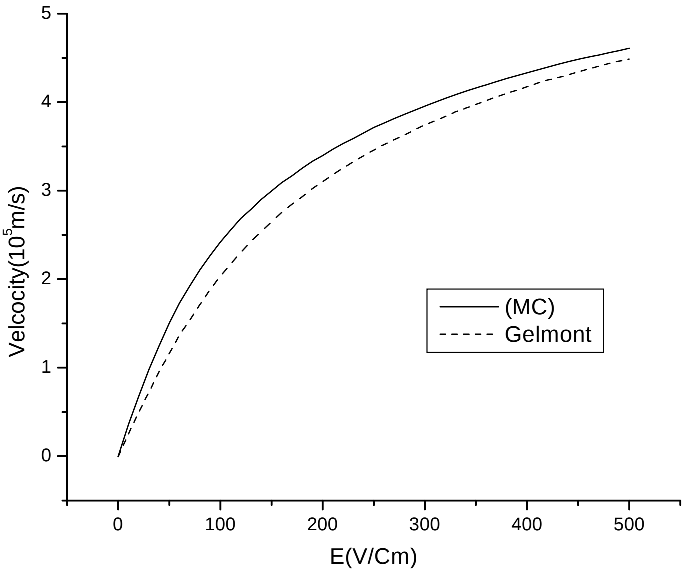

Fig. 2. Profile of the velocity versus electric field E in $Hg_{0.8}Cd_{0.2}Te$.

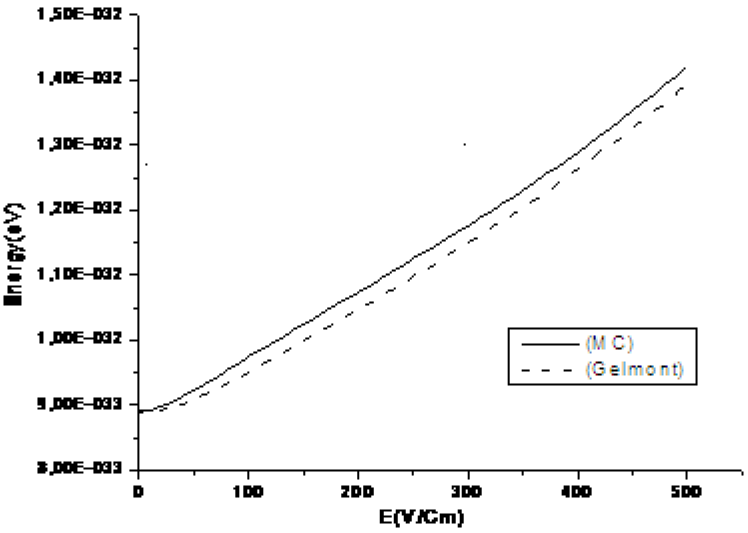

Fig. 3. Evolution of the energy in the electric field E in $Hg_{0.8}Cd_{0.2}Te$.

So the energy exchange between the electron gas and the system will be balanced and the value of the average energy is the thermodynamic equilibrium. Once this field value is exceeded, the holder is an energy that has a linear variation along the field because in this range of fields, collisions are no longer sufficient to dissipate the energy he brings to the electrons, the due to the increase of the average energy, the electron temperature becomes higher than the temperature of the crystal lattice. Everything happens as if the electrons heated more gradually as the electric field increases (regime of hot carriers).

3.2. Nonstationary Mode

We calculated, using Monte Carlo simulation, the speed and the electron energy versus time. To do this, at time t = 0, we applied the system is at thermodynamic equilibrium a step electric field. The results are shown for different values of the electric field in Fig. 4 in terms of speed, and Fig. 5 with respect to energy. Can notice that the speed and energy scribed both a transitional few picoseconds before reaching a stationary value.

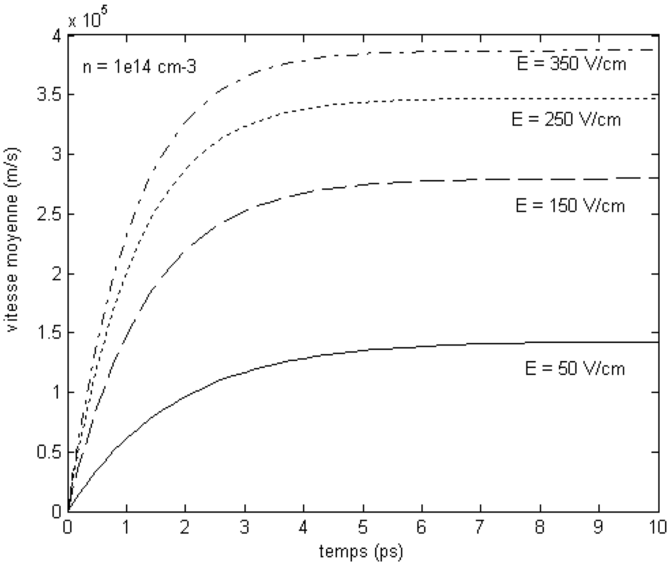

Fig. 4. Electronic speed In function to time for different electric fields.

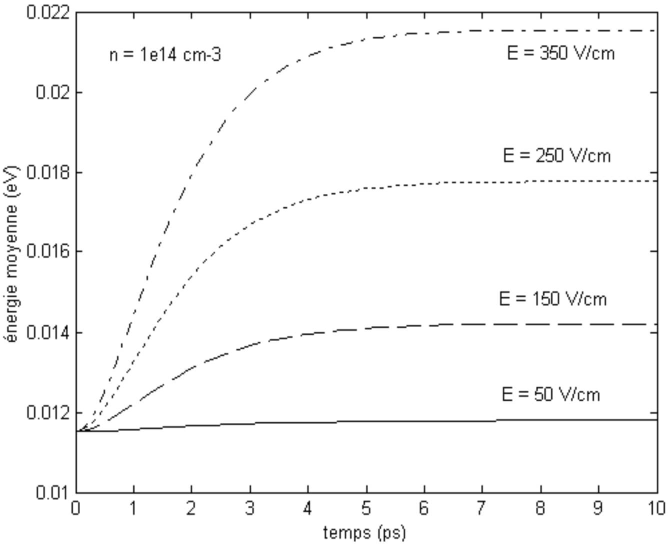

Fig. 5. The energy in function to time for different electric fields.

When the field is sufficiently high, as is the case at 350 V/cm in $Hg_{0.8}Cd_{0.2}Te$, the energy relaxation occurs after electrons have been able to reach values of speed higher than its stationary value, and are emerging during the transient effect of a slight over speed.

3.3. Influence of Doping

Fig. 6: Evolution of energy in the electric field E in $Hg_{0.8}Cd_{0.2}Te$ in different doping.

The effect of coating on the rate of carriers is determined by applying a low field, this effect is illustrated in Fig. 7. It shows the speed variation depending on the field for different concentrations: 10^{14} cm^{-3}, 5.410^{14} cm^{-3} and a curve intrinsic semiconductor. The results show that at low field (50 V / cm) the velocity increases linearly with the field and, for a value of the electric field, this rate is even lower than the density of ionized impurities is important.

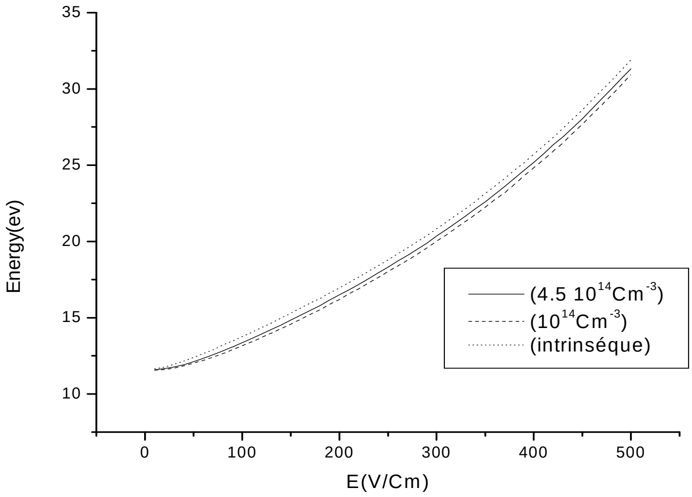

Fig. 6. The energy in function to time for different electric fields.

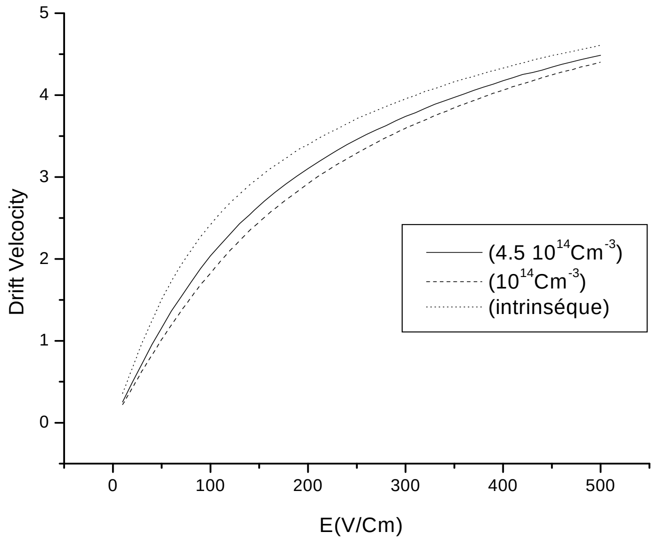

Fig. 7. Evolution of energy in the electric field E $Hg_{0.8}Cd_{0.2}Te$ In different doping.

Once we get field strength above the field of 50 V/cm, the velocity decreases as the doping density increases. It's the fact that when the doping density is increased, the number of carriers increases, hence the number of interactions increases and thus the speed decreases.

Finally the effect of doping is to alternate fields students. Note that the curves converge asymptotically from the time we reached the fields or students.

4. Conclusion

We present results obtained by the Monte Carlo due to the semiconductor $Hg_{0.8}Cd_{0.2}Te$ and we view it is able to describe the transport parameters in steady and unsteady. We highlighted the importance of hot carrier regime that appears in$Hg_{0.8}Cd_{0.2}Te$, from small electric fields. The same applies to the speed of electrons, the latter suffers from the consequences of the regime of hot carriers, and it increases in the electric field. These results are consistent with published experimental results, as well as the numerical ones already published.

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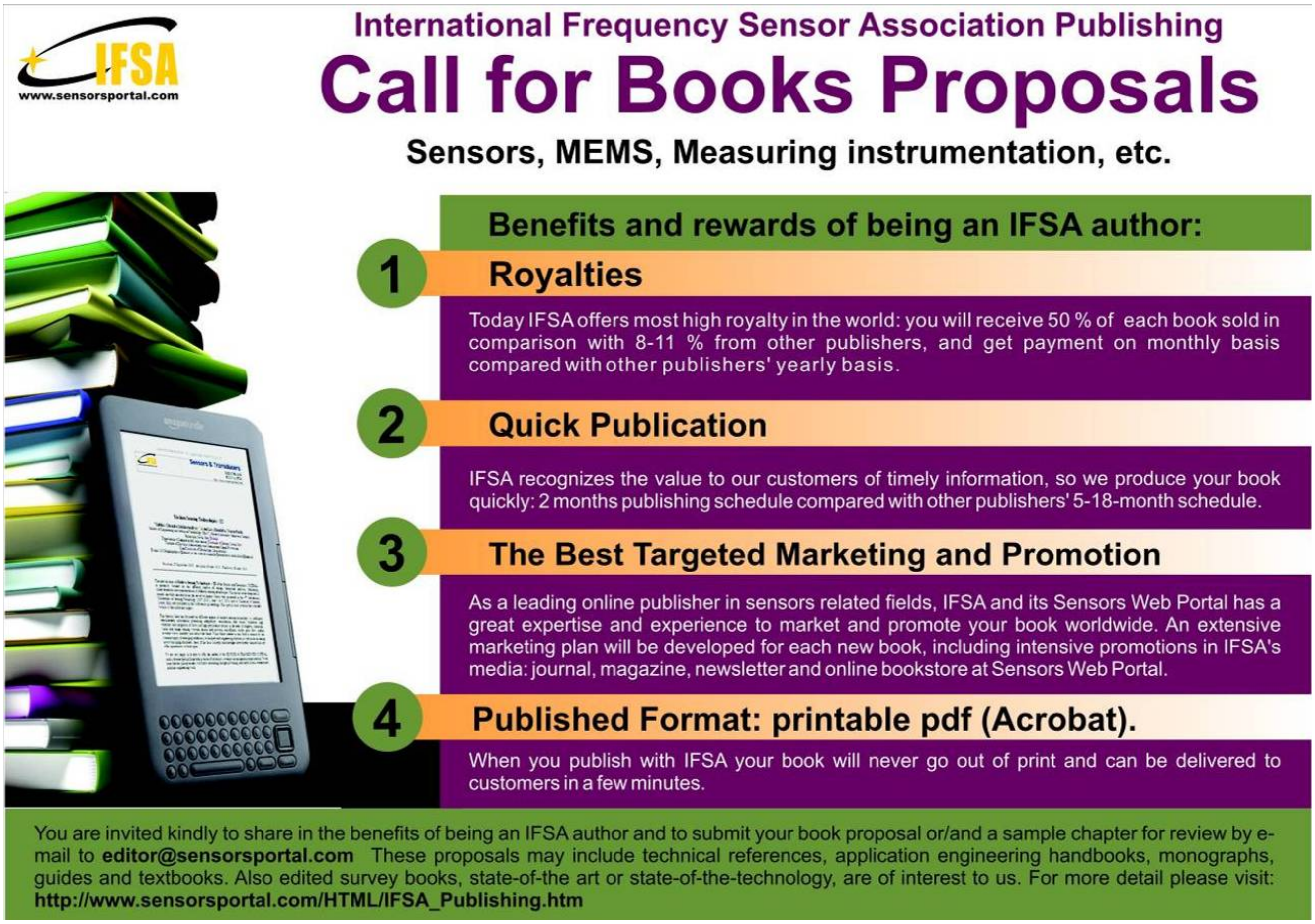

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