

The Study and Simulation of the Electron Transport Phenomena on Bulk $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Based on an Ensemble Monte Carlo Method

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Abstract

In this paper a comparative study of the electronic transport phenomenon in the semiconductor II-VI alloy HgCdTe is presented. In this study we have adopted Monte Carlo simulation. The model of the method used in this work takes into account the valleys, L and X of the conduction band, in which considered isotropic but not parabolic. 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. Furthermore, he permits two main functions: the calculation of the scatterings rates taken into consideration and the determination of the instantaneous quantities such as speed, energy etc. The obtained results, compared on many experimental reference frames, are satisfactory.

Keywords: Monte Carlo simulation; Steady-state electron transport; Transient electron transport; Alloy scattering; Velocity overshoot; Critical field; Interactions; $\text{Hg}_{0.7}\text{Cd}_{0.3}\text{Te}$ alloy

Introduction

Mercury cadmium telluride (HgCdTe) is the material system of choice to fabricate high performance photovoltaic and avalanche detectors over the entire infrared spectral region [1]. Several groups have reported an exponential gain curve and extremely low multiplication noise in electron injected HgCdTe Avalanche Photodetectors (APDs) at temperatures in the range of 77 K to 260 K for a variety of cutoff wavelengths in the MWIR and LWIR bands [2,3]. These exceptional characteristics of HgCdTe APDs are indicative of the exclusive impact ionization of the electrons and of dead-space effects that tend to introduce order in the random impact ionization process, i.e., a history-dependent gain mechanism [4,5]. The electron impact ionization process in HgCdTe becomes important at relatively small electric fields due to the high mobility of electrons and their low impact ionization threshold energy. The high gain at low bias and the low noise factor make HgCdTe APDs particularly well suited for several applications, including night vision, nondestructive control and medical imaging, multicolor focal-plane arrays (FPAs) for astronomy, and photon counting. Despite this interest, a complete description of the transport properties of HgCdTe alloys is still lacking, especially in the high-field regime. The low field mobility has been the only transport parameter that has been the object of extensive theoretical [6] and experimental [7,8] investigations. The electron drift velocity characteristic in CdTe as a function of temperature and electric field was measured by the transient-charge technique by Canali et al. [9] Borsari and coworkers [10] performed Monte Carlo calculations of electron transport in CdTe to investigate the negative differential mobility of this material, which was attributed to the randomizing effect of intervalley scattering rather than to the population of lower-mobility valleys [10].

The current demand growth of new components capable of operating at high power, high frequency, high temperatures and convergence towards miniaturization has lead to the development of new fields of nanotechnology based on II-VI semiconductor. Interest in nanostructures based on II-VI semiconductor narrow gap containing mercury (such as superlattices $\text{HgTe} / \text{CdTe}$) was due to their advantages over alloys with cadmium telluride Mercury (MCT: HgCdTe). The ternary alloy $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is a semiconductor band-gap direct; in our work we are interested in the ternary compound

$\text{Hg}_{0.7}\text{Cd}_{0.3}\text{Te}$. The results obtained are very satisfactory; they are compared with experimental results, and are in good agreement. These results are very promising and open new perspectives for the realization of solar cells and applications in the field of sensors.

Model Description

The most important input to Monte Carlo transport simulation is the electronic structure of the material to be studied [11]. The electronic structures of the binary compounds CdTe and HgTe have been computed by using the Nonlocal Empirical Pseudo Potential Method (NL-EPM), while the ternary alloy HgCdTe has been studied by using NL-EPM within a disorder-corrected Virtual Crystal Approximation (VCA). The computed electronic structures, which take into account spin-orbit interactions, accurately replicate the available experimental data and ab initio information. Figure 1 shows the NL-EPM electronic structure of HgCdTe . The presence of secondary valleys at the L point (intervalley separation energy 1.37 eV) can be noticed. Besides the electronic structure, the carrier-phonon interaction at high energies is the critical piece of information to be evaluated in order to study the carrier dynamics at high fields and impact-ionization-related phenomena. Empirical fits to low-energy transport data are still used to determine the electron-phonon coupling constants, and these values are used for simulation beyond their expected range of validity. The lack of reliable information on the carrier-phonon interaction has always affected the ability to treat the impact ionization process. Scarce information is available on the electron-phonon deformation potentials in HgCdTe . Chattopadhyay and [12] suggested a theoretical

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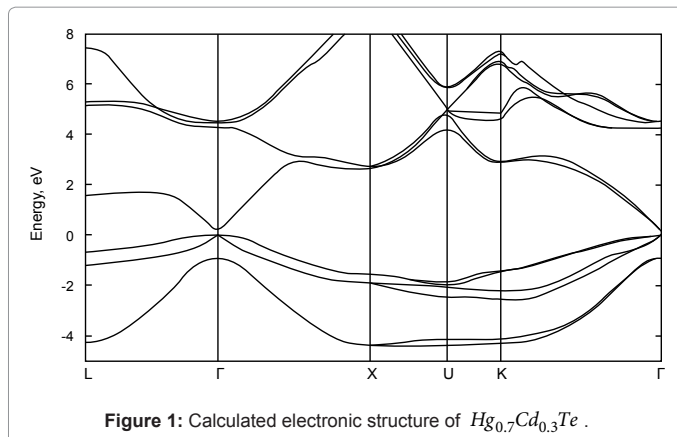


Figure 1: Calculated electronic structure of $\text{Hg}_{0.7}\text{Cd}_{0.3}\text{Te}$.

value of 9.5 eV for the electron acoustic deformation potential in HgCdTe , adopting the value reported by Rode for CdTe [13]. To the authors' knowledge, no information is available for the whole deformation potential coefficients.

The electronic transport is always described by models based on the resolution of the Boltzmann equation who characterizes the modification of the particles state caused by various actions. Thus, 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.

In this work we have to use a three valleys model of the conduction band, Γ , L, X considered isotropic but not parabolic. Our model is developed considering the deformation potential of each considered valley, the energy gap structures, and the main scattering mechanisms in details. The concentrations of electrons in L and X valleys relative to the minimum Γ are:

$$n_{\Gamma} = 2 \left(\frac{2\pi m_{\Gamma}^* K T}{h^2} \right)^{3/2} \exp\left(\frac{E_p}{K T}\right)$$

$$\frac{n_L}{n_{\Gamma}} = \left(\frac{m_{\Gamma}^L}{m_{\Gamma}^{\Gamma}} \right)^{3/2} \exp\left(-\frac{\Delta E_{\Gamma L}}{K T}\right)$$

$$\frac{n_X}{n_{\Gamma}} \left(\frac{m_{\Gamma}^X}{m_{\Gamma}^{\Gamma}} \right)^{3/2} \exp\left(-\frac{\Delta E_{\Gamma X}}{K T}\right) A = \pi r^2$$

Where $E_{\Gamma L}$ and $E_{\Gamma X}$ are the separation energies between Γ -L and Γ -X respectively.

Results

The number of electrons simulated is 20,000 electrons subject to different values of the electric field under different temperatures. The implementation of this model is made by taking the following steps: for each electron simulated, we associate with initial position and an initial wave vector, and using the process "self scattering"; we introduce a fictitious scattering which aims to establish a time distribution.

The Monte Carlo model adopted in this work is used for calculating and retrieval features of electronic transport in the HgCdTe alloy in the

transitional and stationary regime. The calculation is made for electric fields ranging from 0 to 50 KV for different values of temperature.

The average velocity is one of the key parameters to describe the behaviour of a compound. In our study we focus on the modulus of the velocity and the drift velocity is an average velocity of the course. Indeed, the electrons under the influence of thermal energy will have a random way, and therefore they have no path. But when subjected to an electric field their way is more random and the distance travelled is not zero.

After a collision the electron will have a zero velocity component in the direction parallel to the electric field, but the effect of thermal agitation that the electron back to speed, the electrons move in the opposite direction of the field.

In figure 2, we note that the drift velocity increases with the electric field and then it reaches a saturation value equal to $6.16 \cdot 10^7 \text{ Cm/S}$, which corresponds to a critical electric field is 1.2 kV/cm. Thereafter, the drift velocity decreases with the field until it reaches a value of $1.08 \cdot \frac{10^7 \text{ Cm}}{\text{S}}$ from an electric field equal to 14 kV/cm.

In figure 3, when the carriers are subjected to an electric field they will gain energy. We identify two phases, the energy of the three module valleys Γ , L and X. Once the electric field is applied, the energy of the carriers increases very rapidly to a maximum of energy which is 190 meV. After a very short period of time (about 10^{-14}s), we see that the energy becomes constant.

In figure 4, we present the curves for different drift

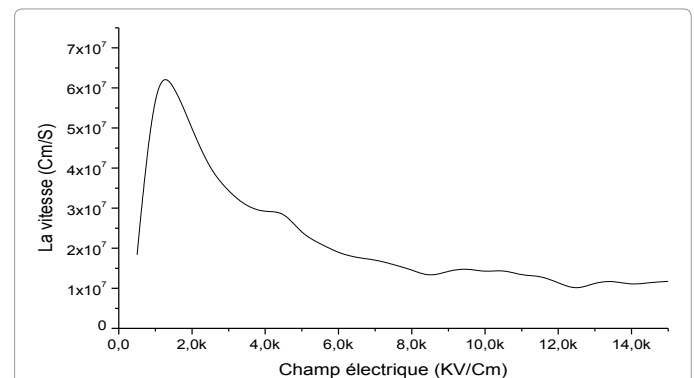


Figure 2: The average velocity in the HgCdTe bulk at 300K for different values of the applied electrical field (Stationary regime).

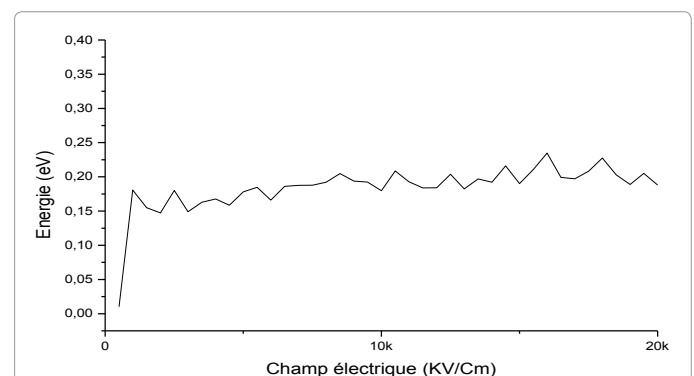


Figure 3: The average energy in the HgCdTe bulk at 300K for different values of the applied electrical field (stationary regime).

velocities in electric fields with time at 300 K. We note that the velocity exhibits a maximum for the strong fields. This is due mainly to the wide variation of angular momentum and energy relaxation as a function of electron energy, so the transient over shoot in velocity is typically observed when the applied electric field is quite high contribution to the critical field; the electrons can reach a maximum energy as the time is small compared to the energy relaxation.

Figure 4 shows the shape of the electron drift velocity versus time for an electric field of 20 kV, and a concentration of $1e^{20}\text{Cm}^{-3}$ at 300 kV. This curve has four phases:

- For $t < 0.2\text{ps}$ the velocity increases linearly with time.
- For $0.2\text{ps} < t < 0.3\text{ps}$ the velocity continues to grow but more slowly. There is a maximum of 1.910^7Cm/s well above the stationary value corresponding to the applied field, so there is a phenomenon of over speed.
- Between 0.3 and 2ps, the velocity decreases rapidly to the steady state.
- In the last phase ($t > 0.9, \frac{10^7\text{Cm}}{\text{s}}$, elocity remains unchanged, it is equal to the steady velocity⁸

When the electrons are subjected to fields largely varying in time, a phenomenon of over-speed 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 5 shows the variation of the drift velocity, energy carriers and the population in the three valleys Γ , L and X with the applied electric field for three different temperatures of the network ($T=200\text{K}$, $T=300\text{K}$ and $T=400\text{K}$), for a mole fraction of $x=0.3$ HgCdTe alloy studied.

At high temperatures, the thermal energy increases, the disorder in the material increases, which implies that collisions at temperature $T=200\text{K}$ with the lattice vibrations are less important than temperature $T=300\text{K}$ and $T=400\text{K}$, by carriers that are subject to thermal agitation disrupts this low and less movement of the carriers.

Conclusion

Research in modeling devices are focused on developing analytical descriptions of the physical devices. In this study we addressed a number

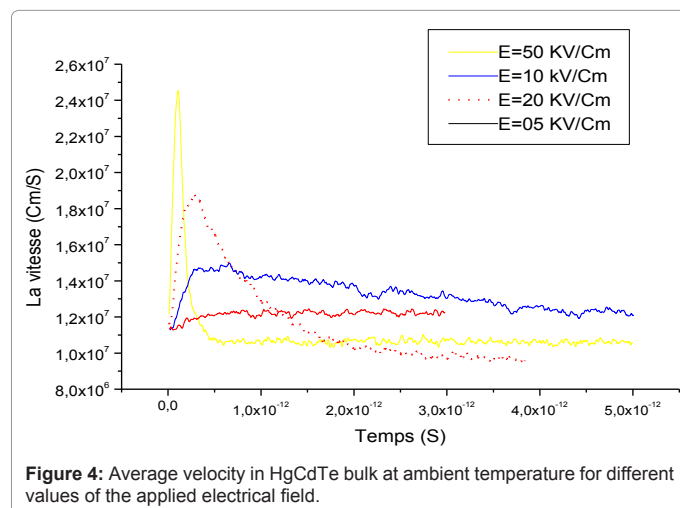


Figure 4: Average velocity in HgCdTe bulk at ambient temperature for different values of the applied electrical field.

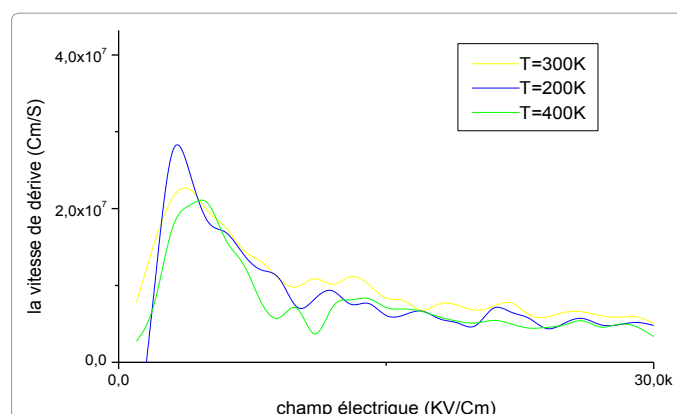


Figure 5: The temperature effect on the drift velocity in HgCdTe bulk with variable electric field.

of issues related to the phenomenon of electron transport carriers in semiconductors II-VI and more precisely in the ternary alloy HgCdTe. We essentially used the program Monte Carlo simulation to describe the functioning of this complex system from the elementary laws governing the movement of electrons. The principle of this approach is to simulate the behavior of electrons in the conduction band using the statistical method of Monte Carlo.

The transient electron transport in the HgCdTe alloy was studied. The characteristics and properties of the material obtained by this model, compared on many experimental reference frames, are satisfactory and they inform us about electronic dynamics as well as the behaviour electric high and low fields and high temperatures of these materials. Furthermore, this results proves the usefulness of this technique as an excellent tool for analysis and simulation of electronic transport phenomena in the semiconductor material, unless the query what is the good definition of physical parameters material which are sometimes poorly understood.

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References

1. Rogalski A (2005) HgCdTe infrared detector material: history, status and outlook. Rep Prog Phys 68: 2267-2336.
2. Kinch MA, Beck JD, Wan CF, Ma F, Campbell J (2004) HgCdTe electron avalanche photodiodes. J Electron Mater 33: 630-639.
3. Derelle S, Bernhardt S, Haidar R, Deschamps J, Primot J, et al. (2009) Experimental Performance and Monte Carlo Modeling of Long Wavelength Infrared Mercury Cadmium Telluride Avalanche Photodiodes. J Electron Mater 38: 1628-1636.
4. Yuan P, Anselm KA, Hu C, Nie H, Lenox C, et al. (1999) A New Look at Impact Ionization—Part II: Gain and Noise in Short Avalanche Photodiodes. IEEE T Electron Dev 46: 1632-1639.
5. McIntyre RJ (1999) A new look at impact ionization-Part I: A theory of gain, noise, breakdown probability, and frequency response. IEEE T Electron Dev 46: 1623-1631.
6. Yoo SD, Kwack KD (1997) Theoretical calculation of electron mobility in HgCdTe. J Appl Phys 81: 719-725.
7. Scott W (1972) Electron Mobility in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. J Appl Phys 43: 1055-1062.
8. Bartoli FJ, Meyer JR, Hoffman CA, Allen RE (1983) Electron mobility in low-temperature $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ under high-intensity CO_2 laser excitation. Phys Rev B 27: 2248-2263.

9. Canali C, Martini M, Ottaviani G (1971) Transport Properties of CdTe. Phys Rev B 4: 422-431.
10. Borsari V, Jacoboni C (1972) Monte Carlo Calculations on Electron Transport in CdTe. Phys Status Solidi B 54: 649-662.
11. Penna M, Marnetto A, Bertazzi F, Bellotti E, Goano M (2009) Empirical Pseudopotential and Full-Brillouin-Zone k-p Electronic Structure of CdTe, HgTe, and $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. J Electron Mater 38: 1717-1725.
12. Chattopadhyay D, Nag BR (1974) Mobility of electrons in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. J Appl Phys 45: 1463-1465.
13. Rode DL (1970) Electron Mobility in II-VI Semiconductors. Phys Rev B 2: 4036-4044.