International Journal of Applied Engineering Research ISSN 0973-4562 Volume 12, Number 7 (2017) pp. 1209-1212

A Comparison between Hydrodynamic and Monte Carlo Model Characteristics of n^+nn^+ Diode Based on $Hg_{0.8}Cd_{0.2}Te$

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Abstract

We performed a One-dimensional ensemble Monte Carlo simulation of a n+nn+ diode based on Hg0.2Cd0.8Te material in comparison with hydrodynamic model. Scattering processes taken into account are polar optical phonon scattering, acoustic phonon scattering, piezo- electric scattering, intervalley phonon scattering, non- polar optical phonon scattering and the ionized impurity scattering. The carrier transport phenomena in the submicron sized device are illustrated by the distribution of over 105 particles in one dimensional device structure. Channel electrons can reach velocities that largely exceed the saturation velocity (velocity overshoot). Such effect guarantees very fast transit times in submicron structures. The electric field is determined self-consistently from the Poisson equation. Numerical results are presented by two models. Based on these data, the excellent agreement of the hydrodynamic approach with Monte Carlo simulations is discussed.

Keywords: Ensemble Monte Carlo, Hydrodynamic, polar optical phonons.

INTRODUCTION

The interest to study electron transport in semiconductor devices at very high electric field has been increased in the last decades (Albrecht et al., 1998). The sub- micrometer structure is one of the most favored devices in the construction of large scale integrated circuits because of its simplicity of construction (Brennan et al., 2002), the comparative lack of doping diffusion problems and the resultant high packing densities possible (O'Leary et al., 2006). Non-equilibrium electron transport aspect in small semiconductor devices have arisen many efforts to improve efficiency of methods that, by solving the Boltzmman transport equation (BTE), deal with the pro- blem of carrier transport at a microscopic level (Bhapkar et al., 1997). The drift diffusion model is not accurate enough to simulate submicrometers semiconductor devices, because it assumes a thermal equilibrium of mean carrier energy (Farahmand et al., 2001; Brennan, 1998).

The approaches based on the hydrodynamic and energy transport balance cannot give a self consistent description of the carrier transport (Fischetti et al., 1991). The microscopic model based on the Monte Carlo method to solve BTE seems to the most adequate for complete study of submicrometers devices (Izuka, 1990; Meinerzhagen et al., 1988).

The transport properties of $Hg_{0.8}Cd_{0.2}Te$ have been extensively investigated in recent years (Sandbom et al., 1989). Currently, this material is used in many electronic and optoelectronic applications such as diodes, solar cells, multispectral photo detection which is of growing interest, in particular to increase targeted discrimination [1]. Hg0.8Cd0.2Te (hereafter indicated as MCT) at a temperature of 77 K, which allows the photo-detection of the 8–14 lm atmospheric window wavelengths. In these conditions, the semiconductor has a narrow band gap of about 100 meV which leads to a strong non-parabolicity of the conduction band and to a small effective electron mass. As a consequence, electron transport properties differ from those of classical semiconductor materials for electronic applications and a high electron mobility, which makes MCT an optimum material for fast applications, is expected. Moreover, physical phenomena such as non-ohmic behavior and impact ionization processes are expected to be of main importance in MCT [2].

In this paper we show that, if the aforementioned problems can be overcome, $Hg_{0.8}Cd_{0.2}Te$ shows every indication that it will ful fill its promise as a useful material. However, simulations for higher anode voltages are needed in view of the situation in practical devices where engineering problems call for anode voltages of no less than about the Schottky barrier height or the p-n junction barrier height. The boundary conditions are important as they have significant influence on the space-charge-limited current flow which become dominant in submicron devices. In recent years, various theoretical approaches have been developed and used to calculate electronic transport characteristics in semiconductor devices. Among these methods the hydrodynamic approach, which combines the simplicity of the drift-diffusion model with the possibility of accounting for non-local effects, such as velocity overshoot, has emerged as a very reliable technique [3]. In general, the hydrodynamic description is

based on velocity and energy conservation equations which are derived from the Boltzmann kinetic equation. However, such a derivation implies the introduction of several assumptions to close the system of conservation equations and, as a consequence, there exists a certain degree of freedom in the choice of the parameters to be used. The aim of this paper is to apply the hydrodynamic model to the case of submicron n+n n+ Hg0.8Cd0.2Te structures.

The comparison between the hydrodynamic model and a Monte Carlo simulation is taken as a validating proof of the hydrodynamic model. In particular, an original decomposition procedure involving the velocity and energy profiles in terms of field, convective and diffusive components has enabled us to carry out a detailed interpretation of electron transport in submicron n+n n+ diode.

SIMULATION METHOD

For a one-dimensional geometry, the hydrodynamic approach model equations consist of the continuity equation.

$$\frac{\partial n}{\partial t}+\nabla\left(n.v\right)=0, \tag{1}$$

The momentum balance equation;

$$\frac{\partial v}{\partial t}+v.\nabla v+\frac{1}{n}.\nabla\left(n.Q_v\right)+\frac{q.\mathrm{E}}{m*}=-\frac{v}{\tau_v}, \tag{2}$$

The energy balance equation.

$$\frac{\partial \varepsilon}{\partial t}+v.\nabla \varepsilon+\frac{1}{n}.\nabla\left(n.Q_\varepsilon\right)+q.\mathrm{E}.v=-\frac{\varepsilon-\varepsilon_0}{\tau_\varepsilon}. \tag{3}$$

Where

$$Q_v\equiv\left\langle\delta v^2\right\rangle=\left\langle v^2\right\rangle-\left\langle v\right\rangle^2$$
$$Q_\varepsilon\equiv\left\langle\delta v\delta\varepsilon\right\rangle=\left\langle v.\varepsilon\right\rangle-\left\langle v\right\rangle.\left\langle\varepsilon\right\rangle \tag{4}$$

where v are the electron density, the electron energy density (average electron energy) and the electron drift velocity, respectively. vx is the x-component of the electron drift velocity and p=m*nv is the momentum density. Corresponding equations are valid for the y and z components. T is the electron temperature and $\mathcal{E}_0$=3/2kT is the average termal equilibrium energy of electrons, where T is the lattice temperature [4].

The electronic current density j inside the active device is

j=nev, so the total current density is

$$\mathrm{j_t}=\text{-nev}+\varepsilon_0\varepsilon_\mathrm{r}\frac{\partial E}{\partial t}. \tag{5}$$

The momentum relaxation time $\mathcal{E}p(\mathcal{E}_0)$ is related to the mobility of the electrons via $\mu(\mathcal{E}_0)=e/m^*(\mathcal{E}_0)\ \tau p(\varepsilon_0)$, and the energy relaxation time $\tau p(\varepsilon_0)$, describes the exchange of energy between the heated electron gas and the lattice. τp, and p=m*nv and the effective electron mass m* are assumed to be functions of the mean electron energy. The hydrodynamic equations, together with Poisson's equation

$$\nabla\left(\varepsilon_{sc}.\mathrm{E}\right)=q\left(n-Nd\right). \tag{6}$$

form a complete set of equations that can be used to solve for the electron density, velocity, energy and electric field for given boundary conditions.

The hydrodynamic model based on equations 1-4 has an evident advantage in that it gives the possibility of verifying directly the assumptions used to close the system of conservation equations. Indeed, the spatial profiles of both velocity and energy can be directly calculated with the Monte Carlo simulation for the structure investigated and compared with those which can be deduced from the hydrodynamic calculations.

Self-consistent Monte Carlo simulation was performed using an analytical band structure model consisting of one non-parabolic ellipsoidal valley [5].

The scattering mechanisms considered in the model are polar scattering by the optical phonons characteristic of CdTe, HgTe and also scattering by ionized impurities and alloy scattering as showing in figure 1.

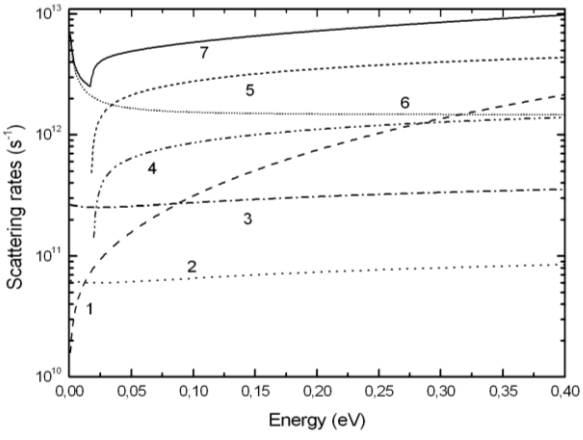

Figure 1: Scattering events in Hg0.8Cd0.2Te occurring in the simulation as function of the energy at 77K. (1) The alloy scattering, (2&3) and (4&5) the optical phonons scattering characteristic of CdTe, HgTe: absorption scattering and emission scattering respectively, (6) ionized impurities scattering and (7) the total scattering.[2]

The overall diode length which is used in both hydrodynamic and Monte Carlo model has 0.6 μm in the x-direction. The parameters of the simulated structure are; the n+ regions are each 0.2 μm thick with a doping density of 5.410^{15} cm-3, the n central region is 0.2 μm of thickness and a doping density

of 10^{14} cm-3. Initially the electrons are in thermal equilibrium with the lattice at T=77K [7]. The carriers' densities are assumed equal to the doping densities (fully ionized impurities).

The applied anode voltage Va is 0.003V, 0.009V and 0.015V to investigate the effects of field variations on the transport properties. This range of voltages is large enough that velocity overshoot and intervalley transfer effects occur.

RESULTS

The electron density and electric field profiles calculated with the hydrodynamic and Monte Carlo models are shown in. Fig. 2 a and b, respectively. An excellent agreement between the results of the 2 approaches is found.

By comparing the value of the electron density through the device, researchers conclude that the electrons diffuse from the cathode and anode into the active layer and are accelerated towards the anode by the field. The resulting space charge causes the departure from a uniform electric field clearly shown in Fig.2b. It is apparent from Fig.2b that both hydrodynamic and Monte Carlo models show that essentially all the potential is dropped in the active layer. However, as a result of the inhomogeneous space charge the field does vary substantially with position, resulting a maximum magnitude near the anode.

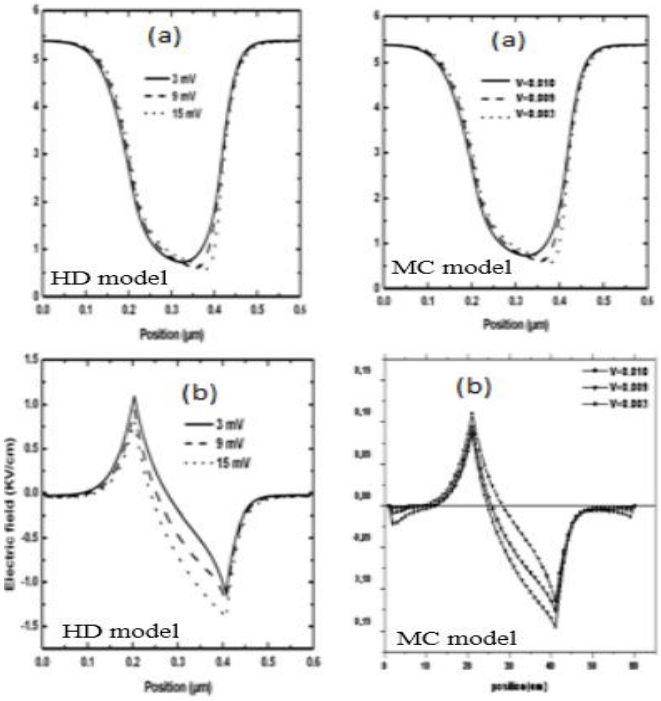

Figure 2. Spatial profiles of electron density and electric field calculated with Monte Carlo and hydrodaynamic approaches for the 0.6 μm $Hg_{0.8}Cd_{0.2}Te$ n^+nn^+ diode with doping levels $n=10^{14}$ m^{-3} and $n^+=5.4$ 10^{15} m^{-3}. The applied anode voltage is varied between 0.003,0.009,0.015 V

As the next step, Fig. 3a and b shows the comparison between the hydrodynamic and Monte Carlo calculations for the velocity and energy profiles.

Even in this case a good agreement between the 2 approaches is achieved. Figure 3a shows that the average drift velocity in the active layer has a maximum value of about $2x10^5$ m sec-1 at 77 K. The plot of average electron km. ethic energy across the device (Fig. 3b) provides further Information on the dynamics. The electrons reach an average energy between 0.14 and 0.16 eV near the anode region and the more energetic electrons in the distribution have sufficient energy to transfer to the upper valleys.

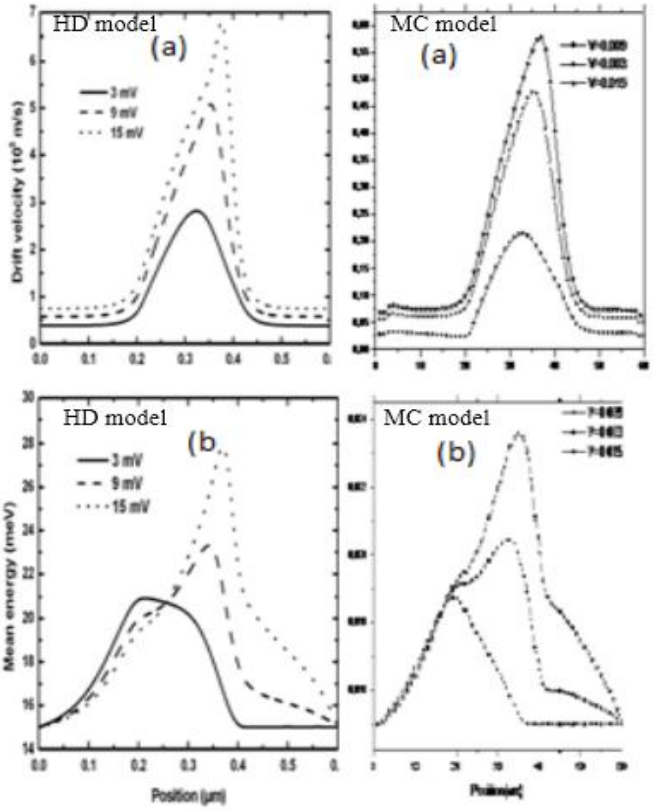

Figure 3: Spatial profiles of (a) drift velocity and (b) electron average energy calculated with Monte Carlo and hydrodynamic approaches for the 0.6 μm Hg0.8Cd0.2Te n+nn+ diode with doping levels $n=10^{14}$ m-3 and $n^+=5.4$ 10^{15} m-3. The applied anode voltage is varied between 0.003,0.009,0.015 V.

CONCLUSION

An ensemble Monte Carlo simulation has been carried out to simulate the electron transport in n+nn+ Hg0.8Cd0.2Te diode at 77 K in comparison with hydrodynamic approach. The hydrodynamic model has been validated by comparison with a Monte Carlo particle simulator. An original decomposition of electron velocity and energy profiles in terms of field, convective and diffusive contributions has

evidenced their importance and their mutual balancing near the homo-junctions. The electrons injected from the cathode initially travel quasi-ballistically but there is substantial transfer to the upper satellite valleys as the anode is approached, resulting in a reduced average electron velocity in that region.

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