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Hydrodynamic simulation of electron transport in n-type $Hg_{0.8}Cd_{0.2}Te$

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Abstract. A hydrodynamic approach based on concentration, velocity and energy conservation equations is developed and used for the simulation of the electron transport in bulk HgCdTe. Both transient and steady-state regimes are simulated using input parameters calculated with a Monte Carlo simulator. The model is validated through a comparison in excellent agreement with Monte Carlo results.

PACS. 67.55.Hc Transport properties – 73.61.Ey III-V semiconductors – 02.70.Uu Applications of Monte Carlo methods

1 Introduction

The first numerical approaches to carrier transport in semiconductors were based on the combination of a drift component due to the applied electric field and a diffusion component due to the concentration gradients [1]: the so-called drift-diffusion approach. However, in the presence of high electric fields, short distances between contacts or short time scales, the drift-diffusion approach loses its validity due to the appearance of hot-carrier and non-local transport effects [2]. In fact, besides carrier density and velocity, also the energy needs to be included in the model since it can differ significantly from the thermal equilibrium value [3,4]: the hydrodynamic (HD) approach, which combines the simplicity of the drift-diffusion model with the possibility of accounting for non-equilibrium effects, has emerged as a very reliable technique. In general, the HD description is based on the solution of a system of coupled differential equations for carrier concentration, velocity and energy conservation equations which are derived from the Boltzmann kinetic equation [5]. 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. On the other hand, the HD approach allows the extraction of important electron parameters by considering in the same framework physical mechanisms of different time scales: for instance, scattering processes and electron generation-recombination phenomena. Among semiconductor materials for which the knowledge of these parameters is fundamental to optimize device performances, we are interested in n-type mercury-cadmium-telluride (HgCdTe) which is a widely used alloy for infrared optoelectronics applications and for which most of these quantities are not well known. The majority of HgCdTe-based devices contain a cadmium fraction $x = 0.2$ which allows, at 77 K, detection in the 8–14 μm spectral region. The consequence of this alloy proportion is a narrow semiconductor band-gap of about 0.1 eV: in particular, degeneracy and impact ionization processes are activated from low electric fields of the order of 100 V/cm [6].

The paper is organized as follows: Section 2 reports the general theory underlying the present HD approach. The results of simulations are presented in Section 3 and the main conclusions are given in Section 4.

2 Hydrodynamic model

For a one-dimensional geometry, the HD modeling of electron transport in semiconductors proposed consists in the following system of conservation equations [5,7]:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(n\nu) = 0 \tag{1}$$

$$\frac{\partial \nu}{\partial t} + \nu\frac{\partial \nu}{\partial x} + m^{*-1}qE = -\frac{\nu}{\tau_\nu} \tag{2}$$

$$\frac{\partial \varepsilon}{\partial t} + \nu\frac{\partial \varepsilon}{\partial x} + qE\varepsilon = -\frac{\varepsilon - \varepsilon_0}{\tau_\varepsilon} \tag{3}$$

where ν is the electron mean velocity, ε the average energy, ε_0 the thermal equilibrium energy, E the electric

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field, q the electron charge, and where τ_ν and τ_ε represent the velocity and energy relaxation times, respectively. In the case of a bulk homogeneous material the unknowns do not depend on space and then spatial derivations can be neglected. Moreover, the electric field E is a constant. Therefore the balance equations reduce to the following form:

$$\frac{\partial n}{\partial t} = 0 \tag{4}$$

$$\frac{\partial \nu}{\partial t} + m^{*-1} qE = -\frac{\nu}{\tau_\nu} \tag{5}$$

$$\frac{\partial \varepsilon}{\partial t} + qE\varepsilon = -\frac{\varepsilon - \varepsilon_0}{\tau_\varepsilon}. \tag{6}$$

This system of equations contains three unknowns which are the electron density n, the mean velocity ν and energy ε. Moreover, it contains three input parameters: the inverse effective mass m^{*-1}, the velocity and energy relaxation times τ_ν and τ_ε, respectively. We remark that the parameters of equations (4)–(6) are, by definition, functions of the mean energy [5,7].

The relaxation times are calculated using the standard balance expressions [7]. The velocity relaxation time is given by:

$$\tau_\nu = \frac{\nu}{qEm^{*-1}} \tag{7}$$

and the energy relaxation time by:

$$\tau_\varepsilon = \frac{\varepsilon - \varepsilon_0}{qE\nu}. \tag{8}$$

In this case we calculate τ_ν and τ_ε using the electron drift velocity and mean energy calculated with a Monte Carlo simulator of the homogeneous material under stationary conditions. For an easier implementation of the energy dependence of the relaxation times in a HD simulator these quantities can be described using the following analytical interpolation formula [8,9]:

$$\nu = \nu_s \frac{E/E_c}{[1 + (E/E_c)]} \tag{9}$$

for the average velocity and:

$$\varepsilon = \varepsilon_0 \left[1 + \left(\frac{E}{E_c}\right)^\beta\right]^\gamma \tag{10}$$

for the average energy. The quantities ν_s and E_c represent the saturation velocity and the critical field, respectively, while β and γ are adjustable parameters.

As concerns the effective mass, we have used the following interpolation formula:

$$m^*(E) = aE^2 + bE + c \tag{11}$$

where a, b and c are adjustable parameters. Finally, we remark that in the HD simulator the dependence of the parameters on the energy is deduced through the electric field dependence of the average energy.

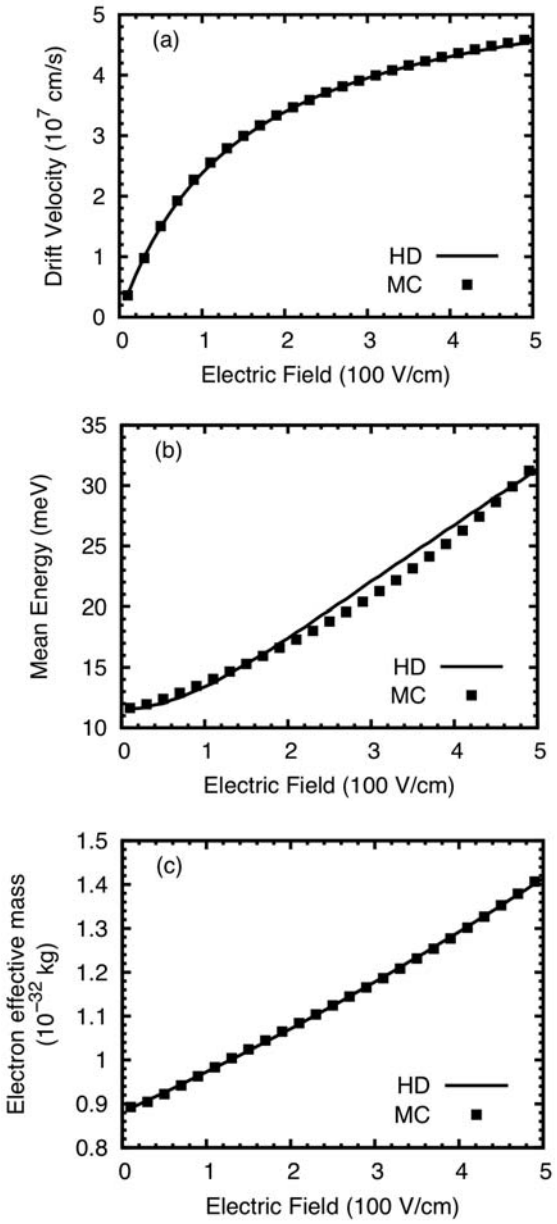

Fig. 1. Velocity (a), energy (b) and effective mass (c) as functions of the applied electric field at 77 K for $Hg_{0.8}Cd_{0.2}Te$ with $n = 10^{14}$ cm^{-3}. Solid lines (HD) refer to analytical expressions and symbols (MC) to Monte Carlo results.

3 Results and discussions

We have reported in Figure 1 the drift velocity (a), mean energy (b) and effective mass (c) as functions of the applied electric field for a concentration $n = 10^{14}$ cm^{-3} at 77 K. The continuous lines refer to relations (9)–(11) whose constants and parameters are given in Table 1, and the symbols refer to Monte Carlo simulations [10]. The drift velocity increases linearly with the electric field up to around 50 V/cm. For higher electric fields, the drift velocity tends to a saturation value around 4.5×10^5 m/s. Indeed, in the range of high electric fields, the transport is dominated by collisions with polar optical phonons. As concerns the energy, it increases monotonously with the

Table 1. Parameters used to express the velocity, mean energy and effective mass analytically for $Hg_{0.8}Cd_{0.2}Te$ with $n = 10^{14}$ cm^{-3} at 77 K.

v_s (10^7 cm/s)	β	γ	E_c (V/cm)	a 10^{-42} Kg m^2 V^2	b 10^{-38} Kg m^2 V^2	c 10^{-32} Kg
5.9	2.20	0.35	148	2.72	9.231	0.953

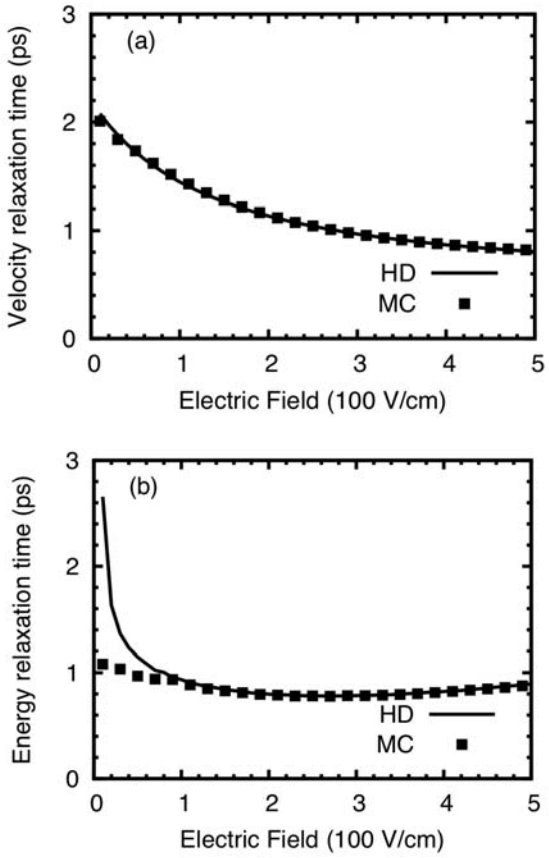

Fig. 2. Velocity (a) and energy (b) relaxation times as functions of the applied electric field at 77 K for $Hg_{0.8}Cd_{0.2}Te$ with $n = 10^{14}$ cm^{-3}. Solid lines (HD) refer to analytical expressions and symbols (MC) to Monte Carlo results.

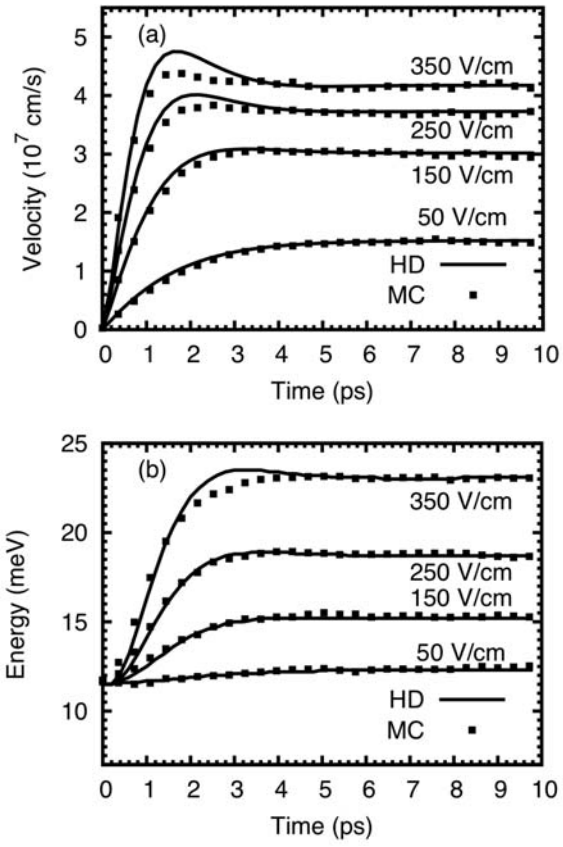

Fig. 3. Mean velocity (a) and energy (b) as functions of time for the reported values of the step-like electric field at 77 K for $Hg_{0.8}Cd_{0.2}Te$ with $n = 10^{14}$ cm^{-3}. Solid lines (HD) refer to hydrodynamic calculations and symbols (MC) to Monte Carlo results.

electric field. We remark that non-ohmic regime is reached for relatively weak electric fields, that is of about 50 V/cm. The high non-parabolicity coefficient of the conduction band (11 eV^{-1}) leads to a small effective mass at low fields of about 0.01 m_0, where m_0 is the free electron mass. On the other hand, the effective mass increases with the electric field of a factor 0.4 between 0 and 500 V/cm. We remark that the analytical formulas allow a quite accurate description of the behavior of the physical quantities calculated with the Monte Carlo simulator.

Figure 2 reports the relaxation time of velocity τ_ν (a) and energy τ_ε (b). As concerns τ_ν, it decreases as a function of the electric field, from 2 to 0.8 ps at 500 V/cm. This behavior results from the increased efficiency of the scattering processes with the electric field. In contrast, τ_ε decreases from 1.1 to 0.8 ps at 250 V/cm and then increases up to 0.9 ps at 500 V/cm. Moreover, we observe that the variation of τ_ε is smaller than that of τ_ν within the considered electric field range. Again, the analytical model reproduces accurately the Monte Carlo results. The discrepancy observed in Figure 2b in the region of very low fields is attributed to the uncertainty in the determination of τ_ε, since both the numerator and the denominator in equation (8) tends to zero when approaching thermodynamic equilibrium.

To complete our investigation, we have calculated the transient regimes of velocity and energy by applying to the system initially at thermodynamic equilibrium a constant step-like electric field. The results are shown in Figure 3 for different values of the electric field. For electric fields

higher than 150 V/cm, the drift velocity exhibits an overshoot higher than the steady-state value. A small overshoot is also detected for the transient energy from fields higher than 250 V/cm. This effect can be attributed to the difference in the velocity and energy relaxation times [9]. Finally we remark that the strong optical phonon scattering in HgCdTe causes the drift velocity and the mean energy to reach their steady-state values in less than 1 ps.

4 Conclusion

Non-equilibrium transport in bulk n-type HgCdTe semiconductor has been successfully modeled using a hydrodynamic semi-classical approach derived from the Boltzmann equation. Using this approach we have calculated the velocity and energy field-dependent relaxation times and modeled the transient behaviors of the average velocity and energy. In all cases, hydrodynamic results have been validated by comparison with calculations performed using the Monte Carlo method.

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