Hydrodynamic modelling of electron transport in submicron Hg$_{0.8}$Cd$_{0.2}$Te diodes

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Abstract. We simulate electron transport in ultra small mercury-cadmium-telluride $n^+\cdot n\cdot n^+$ diodes using a hydrodynamic approach. A numerical staggered solution is employed to treat the coupled hydrodynamic and Poisson equations, where the spatial profiles of the main transport parameters within the diodes are analyzed including the Auger generation-recombination processes. Our numerical results show that, even for low applied voltages, impact ionization processes are activated and affect dramatically the current-voltage characteristics of the Hg$_{0.8}$Cd$_{0.2}$Te diode.

1. Introduction

Carrier transport in advanced submicron devices is not always described with sufficient accuracy by the conventional drift-diffusion (DD) model. As a matter of fact, the DD model does not describe velocity overshoot, diffusion associated with carrier temperature gradients, or the dependence of impact ionization (II) rates on the carrier energy distributions. The limitations of the DD model indicate the need for more general transport models. Two of the more significant classes of such transport models are Monte Carlo (MC) and hydrodynamic (HD). The most accurate kinetic description is given by the MC method because it can take into account explicitly both the energy band-structure and the various scattering phenomena characteristics of the studied material. Therefore it enables a direct calculation of important transport quantities (distribution function, carrier density, drift velocity, mean energy, etc) but at a cost of long computation times and stochastic noise in the output data [1]. On the other hand, the results obtained from the MC simulations permit us also to calculate transport coefficients that can be used as input parameters for more simplified HD models. In this sense, the HD description of electron transport has been extensively applied to the analysis and design of semiconductor devices because it provides a useful compromise between computational simplicity and physical accuracy [2].

In our previous work [3], we have demonstrated the robustness of the HD model to simulate the electronic transport in bulk HgCdTe (Mercury-Cadmium-Telluride, MCT) at 77 K. The majority of MCT-based devices contain a cadmium fraction $x = 0.2$ which allows, at 77 K, the detection in the 8-14 $\mu$m spectral region and which is thus a widely used alloy for infrared optoelectronics applications. 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 [4]. Despite of his wide interest, few results are available in the literature concerning a physical modelling of transport in MCT-based devices. In this paper, we present the simulation of one-dimensional Hg$_{0.8}$Cd$_{0.2}$Te $n^\prime\cdot n\cdot n^\prime$ diodes using the HD approach coupled to the
Poisson equation. The main goal is to investigate the diode electrical behaviour under far-from-equilibrium conditions including the impact ionisation processes.

2. Hydrodynamic transport model

The considered HD model consists of a set of equations expressing the conservation of charge, momentum and energy for each species of carriers. These equations are derived by taking the first three moments of the Boltzmann transport equation. For the one-dimensional case (taking into account the electron-hole generation-recombination processes) these equations take the form [5]:

\[
\frac{\partial n}{\partial t} + \frac{\partial (n\nu)}{\partial x} = g_v n, \tag{1}
\]

\[
\frac{\partial \nu}{\partial t} + \nu \frac{\partial \nu}{\partial x} + \frac{1}{n} \frac{\partial (nQ_v)}{\partial x} + \frac{qE}{m^*} = -\frac{\nu}{\tau_v}, \tag{2}
\]

\[
\frac{\partial \varepsilon}{\partial t} + \nu \frac{\partial \varepsilon}{\partial x} + \frac{1}{n} \frac{\partial (nQ)}{\partial x} + qEV = -\frac{\varepsilon - \varepsilon_c}{\tau_\varepsilon}; \tag{3}
\]

where \( q \) is the absolute value of the electric charge, \( n \) the electron density. The quantities \( \nu, \varepsilon \) represent the average velocity and mean energy, respectively, \( E \) the electric field, \( Q_v \equiv \langle \delta v^2 \rangle = \langle \nu^2 \rangle - \langle \nu \rangle^2 \) the variance of velocity fluctuations and \( Q \equiv \langle \delta v \delta \varepsilon \rangle = \langle \nu \varepsilon \rangle - \langle \nu \rangle \langle \varepsilon \rangle \) the covariance of velocity-energy fluctuations. Still, \( m^* \) is the electron effective mass, \( g_v \) the carrier generation term, and \( \tau_v \) and \( \tau_\varepsilon \) are the momentum and energy relaxation times. For the modelling of voltage driven operation, that is where a constant voltage is applied between the structure terminals, equations (1), (2) and (3) are coupled to the Poisson equation:

\[
\frac{\partial \varepsilon}{\partial x} = \frac{q}{\varepsilon_{sc}} (n - N^+_d) \tag{4}
\]

where \( N_d \) is the ionized donor density and \( \varepsilon_{sc} \) the lattice dielectric constant.

This system of equations contains four unknowns, namely the electron density, the average velocity, mean energy and electric field. Moreover, it contains several input parameters: the effective mass, the velocity and energy relaxation times, the velocity variance and velocity-energy covariance. We note that the parameters of equations (1)-(3) are, by definition, functions of the mean energy and they have been obtained by a previously developed MC simulation of the bulk material under stationary conditions [6].

3. Simulation results

We consider an Hg0.8Cd0.2Te \( n^+\text{-}n\text{-}n^+ \) diode in which the low-doped diode base \( n \) of length \( L \) is sandwiched between two heavily doped contacts \( n^+ \) of length \( d \). The parameters of the simulated structure are: the \( n^+ \) regions are each 0.2 \( \mu m \) thick with a doping density of \( 5.4 \times 10^{15} \text{ cm}^{-3} \), the \( n \) central region is 0.2 \( \mu m \) thick with a doping density of \( 10^{14} \text{ cm}^{-3} \). Initially, the electrons are in thermal equilibrium with the lattice at \( T = 77 \text{ K} \). The carriers densities are assumed to be equal to the doping densities (fully ionized impurities). We present in Figure 1 the carrier density, mean energy, drift velocity and electric field versus position. Three different applied voltages are considered: 12, 15, 21 and 27 mV in order to describe electron behavior from under non-equilibrium conditions.
Figure 1. Stationary profiles accounting for impact ionization of the: (a) electron density, (b) mean energy, (c) drift velocity, (d) electric field as functions of position for a Hg$_{0.8}$Cd$_{0.2}$Te $n^+\,n\,n^+$ diode of length 0.6 $\mu$m for different applied bias at 77 K.

From the simulation results we observe that a significant electron injection is present in the central region due to the diffusion from the $n^+$ regions in conjunction with the quasi-linear variation of the electric field [see Figures 1(a) and 1(d)]. When the voltage applied to the structure increases, the potential barrier in the first $n^+\,n$ homojunction decreases, and the potential mostly drops inside the $n$ region. As a consequence of the fall in the energy barrier, the positive value of the electric field in the first $n^+\,n$ homojunction decreases, and a high negative electric field is found in the active layer ($n$ region), which reaches an extremum of about $-2.1$ kV/cm in the second $n\,n^+$ homojunction. Furthermore, in the $n$ region a significant number of high-energy electrons penetrate in the active layer [see Figure 1(b)]. Therefore, as it can be seen in figure 1(c), the average electron velocity exhibits a significant overshoot reaching a value of $1.1 \times 10^6$ m/s near the high-field region (the saturation velocity in MCT is of the order of $5 \times 10^5$ m/s at 77 K [6]).

The current-voltage characteristics with and without including impact ionization processes for the same structure are shown in Figure 2.
We observe that for the highest considered biases, that is above 21 mV, the impact ionization processes become important and the current density increases rapidly. This behavior is related to the high sensitivity to the bias of Hg\textsubscript{0.8}Cd\textsubscript{0.2}Te material in which generation processes are activated for electric fields much smaller that 1 kV/cm.

4. Conclusion
Device modelling is playing a very important role in the development of semiconductor device design. In this work, a semiconductor device simulator based on the hydrodynamic balance equations has been developed to simulate the electronic transport in Hg\textsubscript{0.8}Cd\textsubscript{0.2}Te \textit{n'}-\textit{n}-\textit{n'} submicron diodes. The numerical results show the presence of hot carrier effects such as the spatial velocity overshoot appearing even for low applied voltages due to the small effective mass characteristic of this material. Moreover, the onset of impact ionization processes, which affects dramatically the current-voltage characteristics, has been put in evidence for relatively small bias voltages with respect to similar devices fabricated with standard semiconductor materials.

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