Theory of Impact Ionization and Auger Recombination in $Hg_{1-x}Cd_xTe$

Boris Gelmont,[a] Ki-Sang Kim, and Michael Shur
Department of Electrical Engineering, University of Virginia, Charlottesville, Virginia 22903-2442
(Received 14 January 1992)

We derived the impact ionization and Auger recombination rates within the framework of the six-band Kane model. The theory involves the electron distribution function and average electron energy which we computed using Monte Carlo simulations, along with the electron drift velocity. The excess carrier concentration is then determined from the balance equation. The results of the calculation are in good agreement with experimental data for HgCdTe at 77 K.

PACS numbers: 79.20.Fv, 72.20.−i

Impact ionization plays an important role in most semiconductor devices. However, the understanding of this phenomenon and, especially, the calculation of the impact ionization rates and current-voltage characteristics under impact ionization conditions is a difficult task because it involves the hot carriers at the energies corresponding to the distribution tail. At such high energies, even the details of the band structure are not usually known with a sufficient degree of accuracy for a quantitative description of the impact ionization, and the band structure cannot be readily described by analytical expressions. This is compounded by numerical difficulties of the calculation of the distribution tail. In this paper, we demonstrate that these difficulties can be successfully resolved for narrow gap semiconductors where the Kane model is accurate enough, the threshold energies of the impact ionization are small compared to the width of the conduction band, and the dominant recombination mechanism is the Auger recombination. In these semiconductors [and, in particular, in mercury cadmium telluride (MCT, $Hg_{1-x}Cd_xTe$, $x\sim0.2$), considered in this paper], the band gap E_g is much smaller than the intervalley separation energies. As a result all processes related to hot electrons are confined within the central valley where the electron wave function and its dispersion law can be described in the frame of the Kane model. This allows us to derive analytical expressions for the impact ionization rate and the rate of the so-called conduction-conduction-heavy-hole-conduction band (CCHC) Auger process.

$Hg_{1-x}Cd_xTe$ has become an important and widely used material of infrared optoelectronics. The most widely used composition with $x=0.2$–0.21 corresponds to the energy gap around 100 meV, and the absorption edge of approximately 12 μm at 77 K. MCT has a very large electron mobility and exhibits a non-Ohmic behavior in relatively small electric fields [1]. The impact ionization becomes important in relatively small electric fields because of the low ionization threshold energy and large electron mobility. Experimental data [1] show that the impact ionization dramatically affects the current-voltage characteristics of the $Hg_{1-x}Cd_xTe$ ($x\sim0.2$) at ~250 V/cm.

First, we calculate the impact ionization rate by electrons, α_n, and the Auger recombination rate R. The particle balance

$$\alpha_n n = Rn^2 p \tag{1}$$

determines the dependence of the carrier concentration on the electric field. Here, electron and hole concentrations, n and p, are linked by the neutrality condition $n=n_0+p$, where n_0 is the electron concentration in the absence of the electric field. Multiplying the carrier concentration by the electron drift velocity, we obtain the current-voltage characteristics which we directly compare with experimental data. Such an approach relies on several approximations. First, it is valid for relatively small hole densities because we do not account for carrier-carrier scattering (see Ref. [2]). However, this is sufficient in order to establish the device behavior near the impact ionization threshold which is the most relevant information for the comparison with the experimental data and or for the device applications. Second, we neglect the impact ionization caused by holes which is justified because, in narrow gap semiconductors, holes remain cold in moderate electric fields causing the impact ionization by electrons. A hot electron transfers almost all its momentum $[\approx 2(m_n E_g)^{1/2}]$ to the created hole whose energy will be of the order $2m_n E_g/m_h$, where m_n and m_h are the electron and heavy-hole effective masses. This value is smaller than the thermal energy at 77 K. Holes are thermalized as a result of subsequent inelastic collisions, primarily with phonons. The electron-hole scattering is not important because of the small ratio of electron and heavy-hole masses. Since the ionization threshold energy, $\varepsilon_t=(2m_n/m_h+1)E_g$, is very close to the energy gap, the final states of both electrons will be near the bottom of the conduction band. Hence, our theory is valid as long as the electron density is much larger than the hole density.

We used the same approach to the calculation of the impact ionization rate and Auger recombination rate for hot electrons as was used by one of us for the theory of the Auger recombination in MCT for cold electrons [3]. The impact ionization rate derived within the framework of the six-band Kane model taking into account the in-

teraction between the s-type conduction band and the fourfold-degenerate-in-the-Γ-point valence band is given by

$$n\alpha_n = \frac{m_n^{5/2} q^4}{4\pi^2 \hbar^6 E_g^{5/2} \kappa^2} \int_{\varepsilon_t}^{\infty} d\varepsilon (\varepsilon - \varepsilon_t)^3 f_c(\varepsilon) , \quad (2)$$

where q is the electron charge, κ is the dielectric constant, $\hbar$ is the Planck constant, and $f_c(\varepsilon)$ is the electron distribution function averaged over angles. According to Eq. (2), the impact ionization rate near threshold is proportional to $(\varepsilon - \varepsilon_t)^3$ and not to $(\varepsilon - \varepsilon_t)^2$ as stated in Ref. [4]. This discrepancy is due to the fact that, in the six-band Kane model, the heavy-hole wave functions are orthogonal to the electron wave functions at the impact ionization threshold. As a result, for the threshold momenta of particles, the overlap integrals vanish. The only nonzero contribution to the overlap integrals comes from the interaction with other bands [3,5]. It was shown in [3], for small m_n/m_h ratios, the quadratic dependence is only valid in the energy interval small compared to $k_B T$. (A more detailed discussion will be given in our future publication.) Our next step was to include the electron heating into the theory of the Auger recombination developed in Ref. [3]. The resulting expression for the Auger recombination rate is given by

$$R = (2\pi)^{5/2} \frac{q^4 \hbar^3 \langle \varepsilon_c \rangle \exp(-2 m_n E_g / m_h k_B T)}{2\kappa^2 m_n^{1/2} E_g^{5/2} (m_h k_B T)^{3/2}} , \quad (3)$$

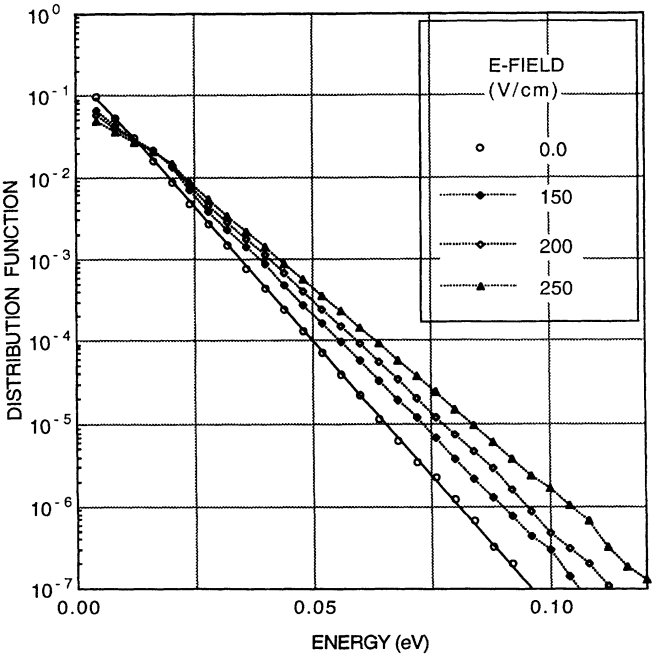

FIG. 1. Distribution functions in $Hg_{0.8}Cd_{0.2}Te$. The solid line for the zero electric field represents the Fermi-Dirac distribution function. The dotted lines are interpolations between computed points.

where $\langle \varepsilon_c \rangle$ is the average electron energy. [Equation (3) is valid for $\langle \varepsilon_c \rangle \ll E_g$.]

We used an ensemble supercomputer Monte Carlo simulation in order to determine the electron distribution function, the average electron energy, and drift velocities in an electric field (see Ref. [6] for a detailed description of our Monte Carlo simulator). We account for polar optical phonon scattering, ionized impurity scattering, and alloy scattering for a nonparabolic band. A detailed derivation of all relevant scattering rates is given in Ref. [7]. We simulated 10000 electrons for 500 time steps of 0.3 ps each. In order to check the accuracy of our Monte Carlo simulation, we first performed the Monte Carlo simulation for zero electric field when we should obtain the Fermi-Dirac distribution function. This simulation showed that our technique is accurate when the distribution function is larger than approximately 2×10^{-7} (see Fig. 1). A typical computed variance of the distribution function in the steady state for the value of the distribution function of 10^{-6} was on the order of 1%. The variation of the computed drift velocity in the steady state was less than 0.1%.

Even for the largest electric fields considered in this paper (250 kV/cm), the estimated scattering rate for the impact ionization ($\approx 10^8$ s^{-1}) is much smaller than the total scattering rate at the threshold ionization energy ($\approx 10^{13}$ s^{-1} at 0.1 eV). Hence, we do not account for the ionization scattering rate in our calculation of the distribution function.

Figure 1 shows the electron distribution functions computed by the Monte Carlo technique for different electric fields. The parameters used in the calculation are given in Ref. [7] where we reported on the Monte Carlo calculation of the drift velocity dependence which showed an excellent agreement with the experimental data [1]. The distribution functions calculated by the Monte Carlo technique and shown in Fig. 1 are accurate near the impact ionization threshold field when the excess carrier concentration does not exceed the electron concentration at zero electric field. Under such conditions, we can neglect the effect of the impact ionization on the electron distribution function. As can be seen from the figure, the distribution function has an exponential asymptotic dependence on energy in the relevant range of the electric fields:

$$f_c(\varepsilon) = A \exp(-\varepsilon / k_B T_{as}) , \quad (4)$$

TABLE I. Parameters of the asymptotic distribution function.

Electric field (V/cm)	$k_B T_{as}$ (meV)	A
150	7.35	0.224
200	7.91	0.169
220	8.28	0.167
235	8.50	0.160
250	8.78	0.159

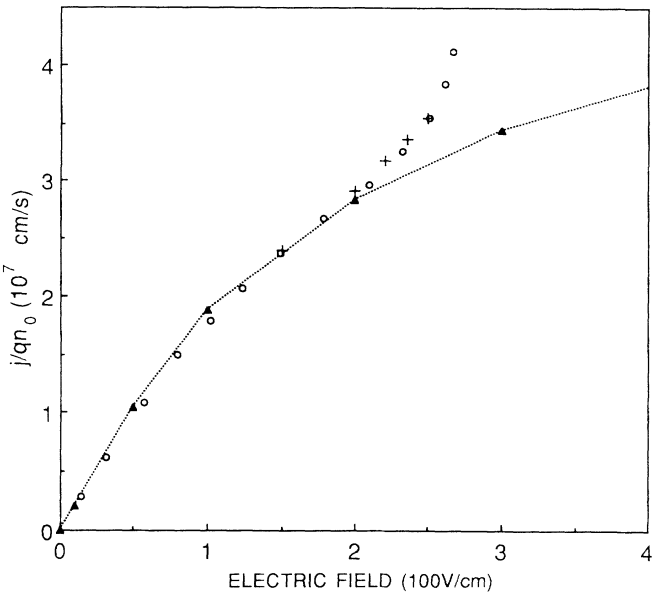

FIG. 2. Calculated and measured normalized current-voltage characteristics of n-type $Hg_{0.8}Cd_{0.2}Te$ sample doped at 5.4×10^{14} cm^{-3} at 77 K. Open circles, experimental data taken from Ref. [1]. Solid triangles and a dotted line, Monte Carlo simulation (no impact ionization included). Crosses, Monte Carlo simulation (impact ionization included).

where constants A and T_{as} depend on the electric field (see Table I). Using Eqs. (2)–(4), we determine the excess carrier concentration from the equation for the particle balance [see Eq. (1)]. The results of the calculation are compared with experimental data in Fig. 2. A good agreement with the experimental data confirms the validity of our approach which can be used for the calculation of the ionization and Auger recombination rates in narrow gap semiconductors and which is simple enough to be implemented in device simulation programs.

This work was supported by the Army Research Office under Contract No. DAL 03-91-G-0048, the Virginia Center of Innovative Technology, and Minnesota Supercomputer Institute.

[a]On leave from A. F. Ioffe Institute of Physics and Technology, St. Petersburg, Russia.

[1] R. Dornhaus, G. Nimtz, and B. Schlicht, *Narrow-Gap Semiconductors* (Springer-Verlag, Berlin, 1983).
[2] P. T. Landsberg, *Recombination in Semiconductors* (Cambridge Univ. Press, Cambridge, 1991).
[3] B. Gelmont, Zh. Eksp. Teor. Fiz. **75**, 536 (1978) [Sov. Phys. JETP **48**, 258–272 (1978)].
[4] B. K. Ridley, *Quantum Processes in Semiconductors* (Clarendon, Oxford, 1988).
[5] B. R. Brennan, J. Appl. Phys. **69**, 7844 (1991).
[6] G. U. Jensen, B. Lund, M. Shur, and T. A. Fjeldly, Comput. Phys. Commun. **67**, 1–61 (1991).
[7] B. Gelmont, B. Lund, K.-S. Kim, G. U. Jensen, M. S. Shur, and T. A. Fjeldly, J. Appl. Phys. **71**, 4977 (1992).