Doping Dependence of Breakdown Field in $Hg_{1-x}Cd_xTe$

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Summary. We apply our theory of the impact ionization and Auger recombination rates in HgCdTe [1] to investigate the dependence of breakdown field on doping. Our calculations show that, in consrast to conventional semiconductors, such as Si or GaAs, the breakdown field is strongly increasing function of the doping concentration.

1. Introduction. $Hg_{1-x}Cd_xTe$ 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 [2]. The impact ionization also becomes important in relatively small electric fields because of the low ionization threshold energy and large electron mobility. Experimental data [2] show that the impact ionization dramatically affects the current-voltage characteristics of the $Hg_{1-x}Cd_xTe$ ($x \sim 0.2$) at ~250 V/cm.

The understanding of the impact ionization 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. As shown in [1] these difficulties can be successfully resolved for narrow gap semiconductors (NGS) such as Mercury Cadmium Telluride (MCT, $Hg_{1-x}Cd_xTe$ ($x \sim 0.2$)). In these semiconductors, the band gap E_g is much smaller than the intervalley separation energies. As a result all processes related to hot electrons are confined to the central valley where the electron wave function and 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 band - Conduction band -Heavy hole band - Conduction band (CCHC) Auger process [1].

2. Ionization rate. According to the Fermi golden rule, the probability of the impact ionization process is given by

$$W = \frac{2\pi}{\hbar V}\sum_{i,f}|g(1,2;h,i) - g(2,1;h,i)|^2 \, f_c(k_i)\delta(\varepsilon_1 + \varepsilon_2 + \varepsilon_h + E_g - \varepsilon_i)$$

$$g(1,2;h,i) = \frac{4\pi q^2 F(1,i)F(2,h)}{(\mathbf{k}_1 - \mathbf{k}_i)^2 \kappa V}$$

where q is the electron charge, κ is the dielectric constant, $\hbar$ is the Planck constant, F is the overlap integral of the lattice periodical parts of the Bloch functions, ε_h is the heavy hole energy, ε_1, ε_2 , k_1 and k_2 are the electron energies and the wave vectors in final state, ε_i and k_i are the electron energy and the wave vector in the initial state, $f_c(k_i)$ is the electron distribution function, V is the volume.

In the Beatty - Landsberg theory, the overlap integrals which are the main parameters of this theory are taken at the threshold energy, ε_t .The logic of the Beatty - Landsberg theory is

based on a certain energy dependence of the overlap integrals and the electron distribution function. The characteristic energy scale for the overlap integrals is of the order of E_g The distribution function changes much more rapidly. Hence, typically, we only need the values of the overlap integrals at the threshold.

Here,we give some details of our derivation of the impact ionization rate for NGS. In the limit of the large spin-orbit splitting energy,only the interaction of six bands is important. If we choose a z-axis along the wave vector k all Bloch wave functions can be written as a superposition of

$$u_{c1}(k) = a_c(k)|S\uparrow> + b_c(k)|1/2> \qquad u_{c2}(k) = a_c(k)|S\downarrow> + b_c(k)|-1/2>$$
$$u_{hh1} = -(X+iY)\uparrow/\sqrt{2} \qquad u_{hh2} = (X-iY)\downarrow/\sqrt{2}$$

where u_{c1} and u_{c2} are electron wave functions, u_{hh1} and u_{hh2} are heavy hole functions, S is the conduction band wave function and X, Y, Z are the valence band functions,and
$|1/2> = [2Z\uparrow - (X+iY)\downarrow]/\sqrt{6}$ $\qquad |-1/2> = [2Z\downarrow + (X-iY)\uparrow]/\sqrt{6}$
are light hole functions at k=0.

The threshold momenta of all particles are parallel to each other. The overlap integrals between the heavy hole and electron wave functions, calculated in the frame of the Kane model, vanish for the threshold momenta of particles since the heavy hole wave functions are orthogonal to the electron wave functions at the threshold. Hence,the overlap integral in NGS is anomalously small at the threshold. Only the interaction with other bands gives a nonzero contribution to the overlap integrals [3,4]. In these materials, the quadratic dependence of the impact ionization rate on energy near the threshold [5] is only valid in an energy interval smaller than the thermal energy, k_BT where k_B is the Boltzmann constant. (This is true for a small ratio of the electron and heavy hole masses m_n/m_h.). This is why the standard theory of the impact ionization rate has to be revised for NGS, and the energy dependence of the overlap integrals has to be taken into account.

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]. In the limit of a small electron average energy in comparison with the forbidden gap, the exchange terms are small and the overlap integrals can be expressed as

$$F_{ch}^2 = 3\hbar^2(\mathbf{k}_2 \times \mathbf{k}_h)^2/(4m_nE_gk_h^2) \qquad F_{cc}^2 = 4/3$$

where k_2 and k_h are the electron and hole wave vectors of the created pair. Introducing the total , $2k$, and relative, k_{12}, wave vectors of electrons in final state, k_1=k-$k_{12}/2$ and k_2=k+$k_{12}/2$, we obtain the following equation for the impact ionization rate

$$n\alpha_n = \frac{(4\pi q^2)^2\hbar^3}{64(2\pi)^8\kappa^2(m_nE_g)^4}\int d^3k_i d^3k_{12} d^3k\{(\mathbf{k}_i\times\mathbf{k}) - (\mathbf{k}_i\times\mathbf{k}_{12})/2\}^2 f_c(\mathbf{k}_i)\delta\{E_g + \frac{\hbar^2}{4m_n}(4k^2+k_{12}^2) + \varepsilon_h(\mathbf{k}_i - 2\mathbf{k}) - \varepsilon_c(\mathbf{k}_i)\} \qquad (1)$$

where ε_c is the electron energy, n is the electron concentration. This equation can be simplified as follows

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

where $\langle f_c(\varepsilon)\rangle$ 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 reference [5]. Our next step was to include the electron heating into the theory of the Auger recombination developed in [3]. The resulting expression for the Auger recombination rate is given by

$$R = (2\pi)^{5/2} \frac{q^4 \hbar^3 < \varepsilon_c > \exp\left(\frac{-2m_n E_g}{m_h k_B T}\right)}{2\kappa^2 m_n^{1/2} E_g^{5/2} (m_h k_B T)^{3/2}} \tag{3}$$

where $\langle \varepsilon_c \rangle$ is the average electron energy. (Eq.(3) is valid for $\langle \varepsilon_c \rangle << E_g$.)

3. Current-voltage characteristics. The dominant recombination mechanism is the Auger recombination. The particle balance

$$\alpha_n = R(n_o + p)p \tag{4}$$

determines the dependence of the carrier concentration on the electric field. Here, p is hole concentration , n_o 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. We used an ensemble 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 non-parabolic band. A detailed derivation of all relevant scattering rates is given in Reference [7]. We simulated 10,000 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. The parameters used in the calculation are given in reference [7] where we reported on the Monte Carlo calculation of the drift velocity dependence which showed an excellent agreement with the experimental data [2]. The distribution functions calculated by the Monte-Carlo technique 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. 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. 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 holes in NGS remain cold in moderate electric fields causing the impact ionization by electrons. A hot electron transfers almost all its momentum ($\approx 2\sqrt{(m_n E_g)}$ where m_n is the electron effective mass) to the created hole whose energy will be of the order $2m_n E_g / m_h$ where m_h is the heavy hole effective mass . This value is smaller than the thermal energy at 77K. 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. The results of the calculation are compared with experimental data in Fig. 1. A very good agreement with the experimental data confirms the validity of our approach which can be

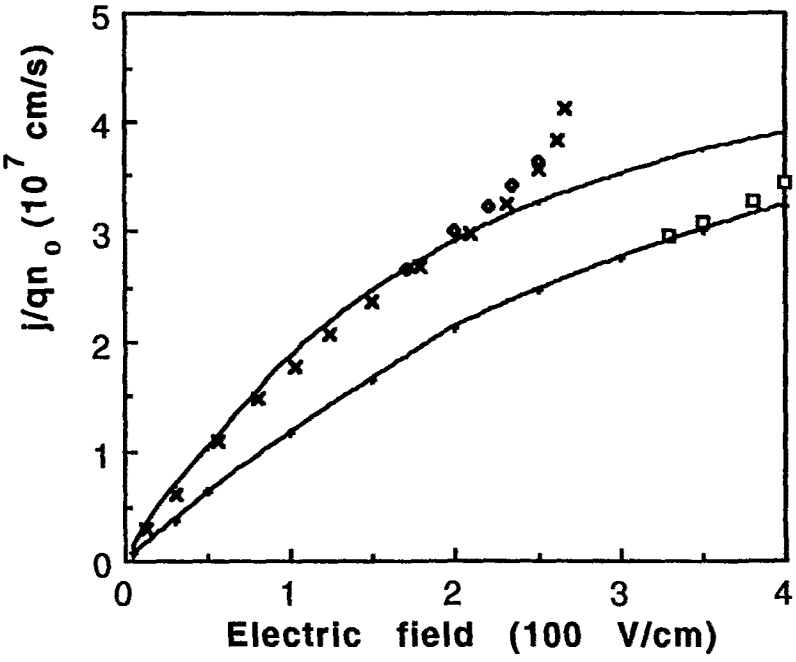

Fig.1.Calculated normalized current-voltage characteristics of n-type $Hg_{0.8}Cd_{0.2}Te$ sample doped at $5.4x10^{14}$ cm^{-3} (diamonds) [1] and at $5.4x10^{15}$ cm^{-3} (squares) at 77 K. Lines are calculations without the impact ionization. Experimental data (crosses) are taken from reference [2].

used for the calculation of the ionization and Auger recombination rates in NGS and which is simple enough to be implemented in device simulation programs.
As can be seen from the figure the breakdown field is higher for a higher carrier concentration whereas in conventional semiconductors, such as Si or GaAs,the breakdown field is practically constant at low doping concentration. The reason for this behavior is that the impact ionization in NGS occurs at low energies , i. e. in the range of energies where the impurity scattering is still important . This result may change a conventional approach to the design of NGS devices where the limitations related to the impact ionization play a dominant role .

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