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A Study of Inelastic Electron-Polar Optical Phonon Scattering in CdTe

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Abstract: The dipolar electric field arising from the opposite displacement of the negatively and positively charged atoms provides a coupling between the electrons and the lattice which results in electron scattering. In this study, a new model of inelastic electron-phonon scattering has been carried out in which the scattering probability does not depend on macroscopic parameter. The reviewed model gives the good agreement between the theory and experiment.

Key words: Dipolar electric field, lattice, electron-phonon scattering, cadmium telluride, parameter, Iran

INTRODUCTION

The dominant scattering mechanism of electrons in polar semiconductors like CdTe comes from the electron-phonon interaction except at the lowest temperatures. The electron-optical phonon interaction contributes both in the ohmic and non-ohmic mobility and provides the dominant energy-loss mechanism of electrons. First order polarization occurs in connection with the primitive unit cell, characteristic of the longitudinally polarized optical mode. In CdTe, the Debye temperature is >1000 K (Welder and Partridge, 1954), hence polar optical phonon scattering must be considered as an inelastic process. Other phonon scattering processes i.e., acoustic and piezo-electric scattering are considered as elastic processes. Like GaAs, CdTe also has a single minimum valley at K = 0 (Γ valley). So, internally phonon scattering can be neglected at low field conditions. In polar optic phonon scattering, the differential scattering rates for absorption and emission can be considered (Smith *et al*., 2002). Also it is found that the electron polar optical phonon scattering rate in CdTe is almost one order of magnitude larger than in GaAs which can be attributed to its larger ionic properties.

THE MODEL OF THE ELECTRON-POLAR OPTICAL PHONON SCATTERING

Let's consider a displacement of j-th atom in a unit cell of a crystal with zincblende structure under the influence of optical oscillations as (Szkatula *et al*., 2002):

$$\mathbf{Q}=\frac{1}{\sqrt{G}}\sum_{\mathbf{q},\nu}\left[\frac{\hbar}{2\,M\,\omega_{\nu}(\mathbf{q})}\right]^{1/2}\left[\xi_j(\mathbf{q},\nu)\,b_{q,\nu}\,e^{i\,\mathbf{q}\rho}+\xi_j^{*}(\mathbf{q},\nu)\,b_{q,\nu}^{*}\,e^{-i\,\mathbf{q}\rho}\right] \quad (1)$$

Where, G is a number of unit cells in a crystal volume; $M = M_{cd}+M_{Te}$ the mass of the unit cell q and $\omega_{\nu}(q)$ wave vector and angular frequency of v-th branch of a crystal optical oscillations, respectively, ξ_j is polarization vector of crystal oscillations; $b_{q,\nu}$ and $b_{q,\nu}^{*}$ operators of phonons annihilation and birth, respectively of v-th branch with wave vector q:

$$\rho = i\,(n_2+n_3)\,\frac{a_0}{2}+j(n_1+n_3)\,\frac{a_0}{2}+k(n_2+n_1)\,\frac{a_0}{2}$$

Under optical oscillations in a unit cell a polarization vector arises:

$$P = \frac{e\,(Q_1-Q_2)}{V_0} \quad (2)$$

Where, $V_0 = a_0/4$ the volume of the unit cell; e-elementary charge Using equation one and taking into account only the long wave ($q\rightarrow 0$) oscillations one can obtain:

$$P=\frac{4\,e}{a_0^3}\sum_{q,\nu}\left[\frac{\hbar}{2\,M\,\omega_{\nu}(q)}\right]^{1/2}(\xi_1(q,\nu)-\xi_2(q,\nu))\times[b_{q,\nu}\,e^{i\,q?}+b_{q,\nu}^{*}\,e^{-i\,q?}] \quad (3)$$

It must be noticed that the polarization vector is a function of discrete variables $P = P(n_1, n_2, n_3)$. To calculate the bound charge ρ = -diveP, let's make following replacement of a partial derivative of a polarization vector on coordinates:

$$\frac{\partial P_x}{\partial x}\rightarrow\frac{P_x(n_1+1,n_2,n_3)-P_x(n_1,n_2,n_3)}{\Delta x}+$$

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$$\frac{P_x(n_1,n_2+1,n_3)-P_x(n_1,n_2,n_3)}{\Delta x}+ \frac{P_x(n_1,n_2,n_3+1)-P_x(n_1,n_2,n_3)}{\Delta x} \quad (4)$$

Where, $\Delta x = a_0/2$ for a unit cell of the zinc blende structure. The similar relations can be written for partial derivatives $\partial P_y/\partial y$ and $\partial P_z/\partial z$ with $\Delta y = \Delta z = a_0/2$. Then poisson equation for a scalar potential bound up with crystal oscillations becomes:

$$\nabla^2\varphi = -\frac{\rho}{\varepsilon_0} = \frac{8\,i\,e}{a_0^{\,3}\varepsilon_0}\sum_q\left[\frac{\hbar}{2\,G\,\omega_v(q)}\right]^{1/2}\times [b_q\,e^{i\,qp}+b_q^{*}\,e^{-i\,qp}] \quad (5)$$

Where, the relation $q_i\,a_0/2<<1 (i = x, y, z)$ is used and only optical longitudinal vibrations are taken into account, ε_0 dielectric constant. To solve the Eq. 5, let's substitute the unit cell by an orb of effective radius $R = \gamma a_0$ the magnitude which lays within the limits from half of smaller diagonal up to half of greater diagonal of a unit cell ($0.5 <\gamma< \sqrt{3}/2$). Magnitude $\gamma = 0.628$ is picked so to adjust the theory with experiment. Spherically, symmetric solution of a poisson equation looks like:

$$\varphi = \frac{\rho}{2\,\varepsilon_0}(R^2-\frac{r}{3}),\ (0\le r\le R) \quad (6)$$

Then, the interaction energy of an electron with polar optical oscillations of a lattice is determined from expression:

$$U = -e\varphi = \frac{4\,i\,e^2}{a_0^{\,3}\varepsilon_0}(R^2-\frac{r}{3})\sum_q\left[\frac{\hbar}{2\,G\,\omega_v(q)}\right]^{1/2}\times \left[b_q\,e^{i\,qp}+\ b_q^{*}\,e^{-i\,qp}\right] \quad (7)$$

Let's mark that the potential Eq. 7 is short-range as it takes into account interaction of an electron only with one unit cell. To calculate the transition probability connected with electron-phonon interaction let's write the wave function of the system electron+phonons in a form:

$$\Psi = \frac{1}{\sqrt{V}}\exp(ikr)\,\Phi(x_1,x_1...x_n) \quad (8)$$

Where, V-crystal volume; $\Phi(x_1, x_1, ...x_n)$ wave function of the system of independent harmonic oscillators. Then, the transition matrix element from interaction energy looks like:

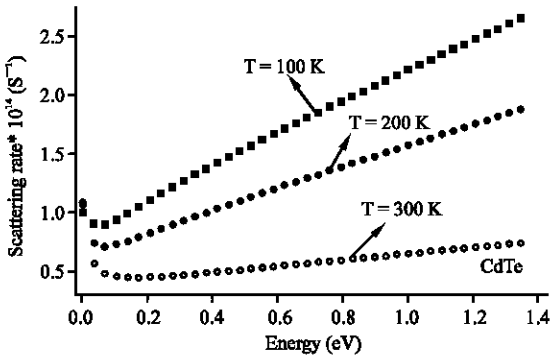

Fig. 1: The dependence of the scattering rate on energy and temperature

$$\langle N_q',k'\,|\,U\,|\,N_q,k\rangle = \frac{4\,i\,e^2}{a_0^{\,3}\varepsilon_0\,V}\int\exp(i\,s\,r)\,(R^2-\frac{r}{3})\times \int\Phi^{*}(x_1,x_1...x_n)\left[\,b_q\,e^{i\,qp}+\ b_q^{*}\,e^{-i\,qp}\right] \Phi(x_1,x_1...x_n)\times dx_1\,dx_2...dx_n,\quad s = k-k' \quad (9)$$

The integration over the electron coordinates is carried out in the limits of unit cell and gives:

$$I(s) = \int\exp(i\,s\,r)\,(R^2-\frac{r}{3})\,dr = \frac{\pi\,(8\,\sin Rs - 8\,Rs\,\cos Rs - 8/3\,R^3s^3\cos Rs)}{s^5} \quad (10)$$

The calculation shows that the electron wave vector (and s together with it) varies within the limits from 0 up to $10^9\,M^{-1}$ at energy changing from 0 up to $10\,k_BT$ at the temperature range 100-300 K. Figure 1 shows the calculated electron-phonon scattering rate versus energy for different temperatures. As indicated, it is shown that with increasing temperature the calculated scattering rate is decreased.

To calculate the sum over the vector q let's do the following simplifications, taking into consideration quasi continuous character of varying of wave vector let's pass from summation to integration over q; let's pass from an integration on a cube with a crossbar $2\pi/a_0$ to an integration on an orb with effective radius π/a_0:

$$\sum_q ... \to \frac{V}{(2\pi)^3}\int_{-\pi/a_0}^{\pi/a_0}\int_{-\pi/a_0}^{\pi/a_0}\int_{-\pi/a_0}^{\pi/a_0} ...\,dq_x dq_y dq_z \to \int_0^{2\pi}\int_0^{\pi}\int_0^{\pi/a_0} ...q^2\sin\theta\,dq\,d\theta\,d\varphi \quad (11)$$

Then, we obtain for the sum the following expression:

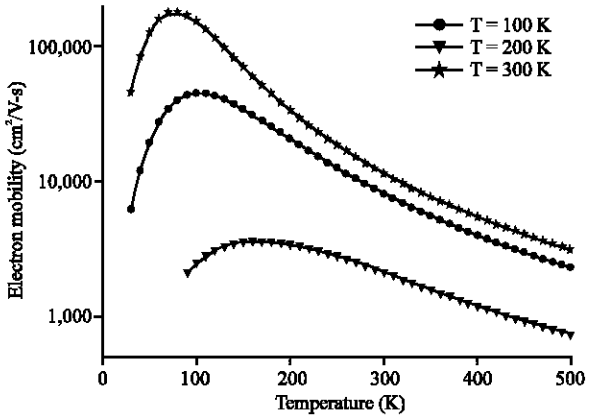

Fig. 2: The temperature dependence of electron mobility in CdTe

$$\sum_q ... = F(\rho) = \pi \frac{4\rho^2 Q^2 \cos \rho Q - 8 \quad 8 \cos \rho Q + 8 \rho Q \sin \rho Q -}{\rho^4} \times$$

$$\begin{cases} \sqrt{N_q} - \text{absorption;} \\ \sqrt{N_q + 1} - \text{radiation, } Q = \pi / a_0 \end{cases}$$

Where, ε is the electron energy. On the base of this forintra and interband electron transitions, the values $K^{nm}_{\beta\alpha a b}$ figuring in a method of a precise solution of the stationary Boltzmann equation can be obtained (Szkatula *et al*., 2002; Pilipenko, 1991):

$$K^{nm}_{\beta\alpha 11} = -\frac{2V}{(2\pi)^3} \frac{64\,\pi^6 e^4 \hbar^2 \gamma^{10}}{675\,\varepsilon_0^{\,2} a_0\, \omega_0 k_B T} \frac{M_{Hg} + M_{Te}}{M_{Hg} M_{Te}} \delta_{\alpha\beta} \times$$

$$\int \{ N_q f_0(\varepsilon) \left[1 - f_0(\varepsilon + \hbar\omega_0)\right] k^2(\varepsilon + \hbar\omega_0) \times$$

$$\frac{\partial k(\varepsilon + \hbar\omega_0)}{\partial \varepsilon} + (N_q + 1)\, \theta(\varepsilon - \hbar\omega_0) f_0(\varepsilon) \times$$

$$\left[1 - f_0(\varepsilon - \hbar\omega_0)\right] k^2(\varepsilon - \hbar\omega_0) \frac{\partial k(\varepsilon - \hbar\omega_0)}{\partial \varepsilon} \Big\} k^4(\varepsilon) \times$$

$$\left(\frac{2\, m_{hh}}{\hbar^2}\right)^{3/2} \delta_{\alpha\beta} \int (N_q + 1) f_0(\varepsilon) \left[1 - f_0(\varepsilon - \hbar\omega_0)\right] \times$$

$$(-\varepsilon - \varepsilon_g + \hbar\omega_0)^{1/2} k^4(\varepsilon) \frac{\partial k(\varepsilon)}{\partial \varepsilon} \varepsilon^{n+m} d\varepsilon$$

Where, $\delta_{\alpha\beta}$ Kronecker delta; $f_0(\varepsilon)$ Fermi-Dirac function; $\theta(x)$-step function. The calculation of the temperature dependence of electron mobility was made for acceptor concentration $N_A = 3\times10^{15}$ cm^{-3}, thus it is possible to neglect the contribution of heavy holes (about 1%). At calculations, the same scattering mechanisms (Szkatula *et al*., 2002; Pilipenko, 1991; Donaldson, 1990) were taken into consideration. As it shown from Fig. 2, the theoretical curve well coincides with experimental data at the temperature range T>100 K. It testifies that the model, offered by us, adequately describes the electron-polar optical phonon scattering process as against model introduced (Welder and Partridge, 1954). From Fig. 2, it is also seen that the basic scattering mechanism in the interval T>100 K is intraband scattering on polar optical phonons. The contribution of the interband scattering is negligible and can be neglected.

CONCLUSION

The model of inelastic electron-polar optical phonon scattering in CdTe is designed which in the framework of a precise solution of the stationary Boltzmann equation well coincides with experiment at the temperature range T>100 K.

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