

INELASTIC ELECTRON SCATTERING BY POLAR OPTICAL PHONONS IN MERCURY TELLURIDE

O.P. MALYK

UDC 621.315.592
© 2004

National University "L'vivska Politekhnik" (12, St. Bandera Str., Lviv 79013, Ukraine; e-mail: malyk@mail.lviv.ua)

A model of inelastic electron scattering by polar optical phonons (ESPOP) is proposed in which the scattering probability does not depend on a microscopic parameter, the crystal permittivity. The model considered gives a good agreement between the theory and experiment in the temperature range 77 – 300 K.

ESPOP in HgTe in the relaxation-time approximation has been considered in works [1, 2]. In [3], this scattering mechanism was considered with taking into account its inelasticity within the frame of the accurate solution of the Boltzmann stationary equation. Ibidem it was shown that the application of the standard ESPOP model leads to a discrepancy between the theory and experiment for temperatures above 100 K. In our thought, this model possesses the following drawbacks: i) it uses a microscopic parameter of crystal permittivity that is of no sense in microscopic processes; ii) the potential of interaction between an electron and a crystal's optical oscillation is a long-range one, thus being in contradiction with the special relativity. The objective of this work is the construction of a scattering model that, firstly, would be in good agreement with experimental data and, secondly, eliminate the above-mentioned drawbacks.

ESPOP Model

Let us consider an optical-oscillation-induced displacement of the j -th atom ($j = 1, 2$) in the elementary cell of a crystal possessing the zinc blende structure [4]

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

where G is the number of elementary cells comprised in the crystal volume; $M = M_{\text{Hg}} + M_{\text{Te}}$ — mass of the elementary cell; \vec{q} and $\omega_\nu(\vec{q})$ are, respectively, the

wave vector and the angular frequency of the ν -th branch of crystal's optical oscillations ($\nu = 4, 5, 6$); $\vec{\xi}_j$ — polarization vector of crystal's oscillations; $b_{\vec{q}, \nu}$ and $b_{\vec{q}, \nu}^*$ — operators of annihilation and creation of photons of the ν -th branch with wave vector \vec{q} ; $\vec{\rho} = \vec{i}(n_2 + n_3)\frac{a_0}{2} + \vec{j}(n_1 + n_3)\frac{a_0}{2} + \vec{k}(n_2 + n_1)\frac{a_0}{2}$, ($n_1, n_2, n_3 = 1, 2, \dots$), a_0 — the lattice constant; $\vec{i}, \vec{j}, \vec{k}$ — the unit vectors of the main axes of the crystal.

Optical oscillations inside the unit cell give rise to a polarization vector

$$\vec{P} = \frac{e(\vec{Q}_1 - \vec{Q}_2)}{V_0}, \quad (2)$$

where $V_0 = a_0^3/4$ is the volume of the unit cell, e — the elementary charge. Using Eq. (1) and taking into account only long-wave ($\vec{q} \rightarrow 0$) oscillations, we obtain

$$\vec{P} = \frac{4e}{a_0^3} \sum_{\vec{q}, \nu} \left[\frac{\hbar}{2GM\omega_\nu(\vec{q})} \right]^{1/2} (\vec{\xi}_1(\vec{q}, \nu) - \vec{\xi}_2(\vec{q}, \nu)) [b_{\vec{q}, \nu} e^{i\vec{q}\vec{\rho}} + b_{\vec{q}, \nu}^* e^{-i\vec{q}\vec{\rho}}]. \quad (3)$$

Note the polarization vector is a function of discrete variables $\vec{P} = \vec{P}(n_1, n_2, n_3)$. To calculate the bound charge $\Lambda = -\text{div}\vec{P}$, let us make the following substitution of the partial derivative of the polarization vector with respect to a coordinate:

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

where $\Delta x = a_0/2$ characterizes the unit cell of the zinc blende structure.

A similar expression can be written for the derivatives $\frac{\partial P_y}{\partial y}$ and $\frac{\partial P_z}{\partial z}$ with $\Delta y = \Delta z = \frac{a_0}{2}$.

Then the Poisson equation for scalar potential φ connected with vibrations of the crystal takes a form

$$\begin{aligned} \nabla^2 \varphi = -\frac{\Lambda}{\varepsilon_0} = \frac{8ie}{a_0^3 \varepsilon_0} \sum_{\vec{q}} \left[\frac{\hbar}{2G\omega_\nu(\vec{q})} \right]^{1/2} \times \\ \times \left[\frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} \right]^{1/2} \frac{(q_x + q_y + q_z)^2}{q} [b_{\vec{q}} e^{i\vec{q}\vec{\rho}} - b_{\vec{q}}^* e^{-i\vec{q}\vec{\rho}}], \end{aligned} \quad (5)$$

where we use the relation $q_i \frac{a_0}{2} \ll 1$ ($i = x, y, z$) and take into account the longitudinal optical vibrations only; ε_0 is the dielectric constant.

To solve Eq. (5), let us replace the unit cell with a sphere of effective radius $R = \gamma a_0$ falling into the interval between a half of the smaller cell's diagonal and that of the larger one ($0.5 < \gamma < \sqrt{3}/2$). To achieve a correspondence between the theory and the experiment, we take $\gamma = 0.628$. The spherically symmetric solution of Eq. (5) is written as

$$\varphi = \frac{\Lambda}{2\varepsilon_0} \left(R^2 - \frac{r^2}{3} \right), \quad (0 \leq r \leq R). \quad (6)$$

In this case, the energy of electron interaction with polar optical oscillations of the lattice can be found from the expression

$$\begin{aligned} U = -e\varphi = \frac{4ie^2}{a_0^3 \varepsilon_0} \left(R^2 - \frac{r^2}{3} \right) \sum_{\vec{q}} \left[\frac{\hbar}{2G\omega_\nu(\vec{q})} \right]^{1/2} \times \\ \times \left[\frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} \right]^{1/2} \frac{(q_x + q_y + q_z)^2}{q} [b_{\vec{q}} e^{i\vec{q}\vec{\rho}} - b_{\vec{q}}^* e^{-i\vec{q}\vec{\rho}}]. \end{aligned} \quad (7)$$

Note that potential (7) is a short-acting one since it takes into account the electron interaction with a single unit cell. To calculate a probability of the electron-phonon-interaction-associated transition, let us write a wave function of the "electron + phonons" system in the following form:

$$\Psi = \frac{1}{\sqrt{V}} \exp(i\vec{k}\vec{r}) \Phi(x_1, x_2 \dots x_n), \quad (8)$$

where V is the crystal volume, $\Phi(x_1, x_2 \dots x_n)$ — wave function of the system of non-interacting simple oscillators.

Then, the matrix element of the interaction energy takes form

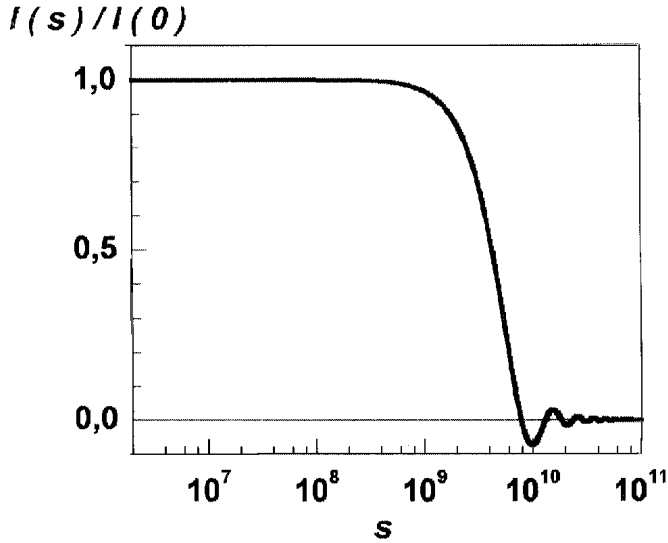
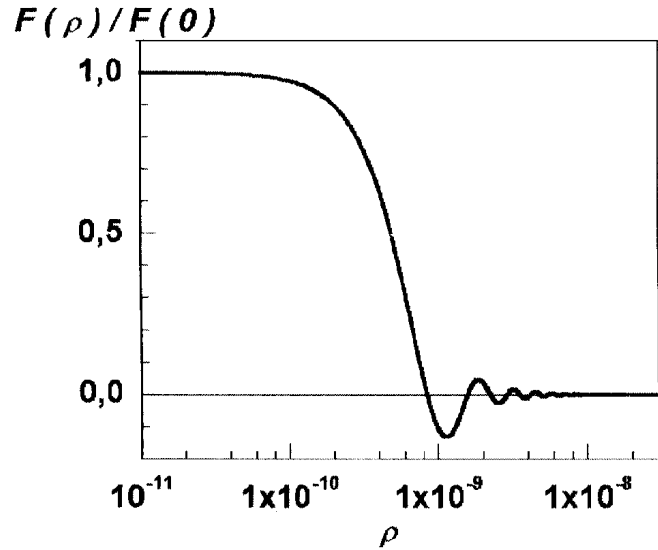
$$\begin{aligned} \langle N'_{\vec{q}}, \vec{k}' | U | N_{\vec{q}}, \vec{k} \rangle = \frac{4ie^2}{a_0^3 \varepsilon_0 V} \times \\ \times \int \exp(i\vec{s}\vec{r}) \left(R^2 - \frac{r^2}{3} \right) d\vec{r} \sum_{\vec{q}} \left[\frac{\hbar}{2G\omega_\nu(\vec{q})} \right]^{1/2} \times \\ \times \left[\frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} \right]^{1/2} \frac{(q_x + q_y + q_z)^2}{q} \times \\ \times \int \Phi^*(x_1, x_2 \dots x_n) [b_{\vec{q}} e^{i\vec{q}\vec{\rho}} - b_{\vec{q}}^* e^{-i\vec{q}\vec{\rho}}] \times \\ \times \Phi(x_1, x_2 \dots x_n) dx_1 dx_2 \dots dx_n, \quad \vec{s} = \vec{k} - \vec{k}'. \end{aligned} \quad (9)$$

Integration over the electron coordinates is accomplished within the limits of the unit cell and results in

$$\begin{aligned} I(s) = \int \exp(i\vec{s}\vec{r}) \left(R^2 - \frac{r^2}{3} \right) d\vec{r} = \\ = \frac{\pi(8 \sin Rs - 8Rs \cos Rs - 8/3 R^3 s^3 \cos Rs)}{s^5}. \end{aligned} \quad (10)$$

As the calculation shows, the wave vector of an electron (along with the s value) changes within the interval from 0 to 10^9 m^{-1} if the energy changes from 0 to $10 k_B T$ (k_B is the Boltzmann constant) in the temperature range 4.2 — 300 K. From the dependence of $I(s)/I(0)$ on s , presented in Fig. 1, it is seen that the relationship $I(s) \approx I(0) = 16/15\pi R^5 = 16/15\pi a_0^5 \gamma^5$ is satisfied sufficiently well within the mentioned limits of the wave vector variation.

The integration over the coordinates of harmonic oscillators gives the factors $\sqrt{N_{\vec{q}}}$ and $\sqrt{N_{\vec{q}} + 1}$ (with $N_{\vec{q}}$ being the number of photons with frequency $\omega(\vec{q}) = \omega_0$ at $\vec{q} \rightarrow 0$) for the operators of annihilation and creation, correspondingly. To accomplish the summation over the vector \vec{q} , we make the following assumptions: i) taking into account the quasi-continuous type of the wave vector variation, we pass from the summation to integration with respect to \vec{q} ; and ii) we pass from the integration over a $2\pi/a_0$ -edge cube to the integration


 Fig. 1. Dependence of $I(s)/I(0)$ on $s = |\vec{k} - \vec{k}'|$

 Fig. 2. Dependence of the function $I(\rho)/I(0)$ on ρ

over a sphere of effective radius π/a_0 :

$$\begin{aligned} \sum_{\vec{q}} \dots &\rightarrow \frac{V}{(2\pi)^3} \int_{-\pi/a_0}^{\pi/a_0} \int_{-\pi/a_0}^{\pi/a_0} \int_{-\pi/a_0}^{\pi/a_0} \dots dq_x dq_y dq_z \rightarrow \\ &\rightarrow \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi/a_0} \dots q^2 \sin \theta d\theta d\varphi. \end{aligned} \quad (11)$$

Then, we obtain the following expression for the sum:

$$\begin{aligned} \sum_{\vec{q}} \dots &= F(\rho) = \\ &= \pi \frac{8 \cos \rho Q + 8 \rho Q \sin \rho Q - 4 \rho^2 Q^2 \cos \rho Q - 8}{\rho^4} \times \\ &\times \begin{cases} \sqrt{N_{\vec{q}}} - \text{absorption;} \\ \sqrt{N_{\vec{q}} + 1} - \text{emission. } Q = \pi/a_0. \end{cases} \end{aligned} \quad (12)$$

From the dependence $F(\rho)/F(0)$ vs ρ presented in Fig. 2, it is seen that the function $F(\rho)$ can be approximated by the expression

$$F(0) = \pi Q^4 \times \begin{cases} \sqrt{N_{\vec{q}}} \\ \sqrt{N_{\vec{q}} + 1} \end{cases}. \quad (12a)$$

After calculations, we obtain the probability of the electron transition connected with the phonon absorption/emission:

$$\begin{aligned} W(\vec{k}, \vec{k}') &= \frac{64\pi^7 \gamma^{10} e^4}{225 \varepsilon_0^2 a_0^4 G \omega_0} \frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} [N_{\vec{q}} \delta(\varepsilon' - \varepsilon - \\ &- \hbar \omega_0) + (N_{\vec{q}} + 1) \delta(\varepsilon' - \varepsilon + \hbar \omega_0)] \end{aligned} \quad (13)$$

with ε being the electron energy.

Basing on this result, we can calculate the values $K_{\beta\alpha ab}^{nm}$ for intra- and inter-zone transitions of an electron; these values appear in the method of exact solution of the stationary Boltzmann equation [3]:

$$\begin{aligned} K_{\beta\alpha 11}^{nm} &= -\frac{2V}{(2\pi)^3} \frac{64\pi^6 e^4 \hbar^2 \gamma^{10}}{675 \varepsilon_0^2 a_0 \omega_0 k_B T} \times \\ &\times \frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} \delta_{\alpha\beta} \int \left\{ N_{\vec{q}} f_0(\varepsilon) [1 - f_0(\varepsilon + \hbar \omega_0)] \times \right. \\ &\times k^2(\varepsilon + \hbar \omega_0) \frac{\partial k(\varepsilon + \hbar \omega_0)}{\partial \varepsilon} + \\ &+ (N_{\vec{q}} + 1) \theta(\varepsilon - \hbar \omega_0) f_0(\varepsilon) [1 - f_0(\varepsilon - \hbar \omega_0)] \times \\ &\left. \times k^2(\varepsilon - \hbar \omega_0) \frac{\partial k(\varepsilon - \hbar \omega_0)}{\partial \varepsilon} \right\} k^4(\varepsilon) \frac{\partial k(\varepsilon)}{\partial \varepsilon} \varepsilon^{n+m} d\varepsilon; \end{aligned}$$

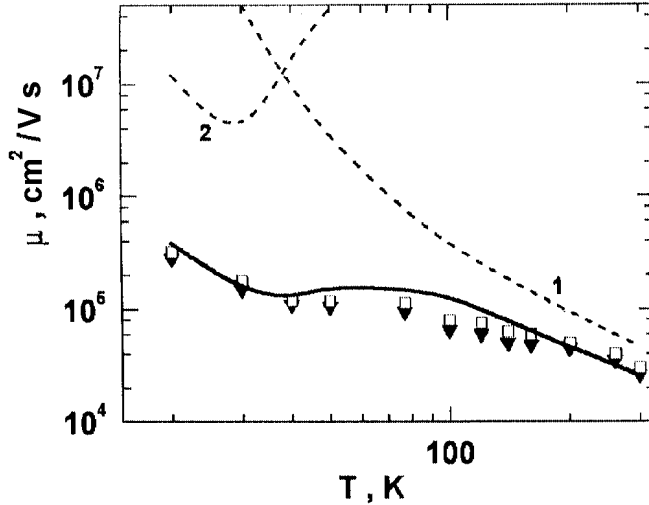


Fig. 3. Dependence of electrons' mobility on temperature in HgTe: solid line shows the action of the mixed scattering mechanism; 1 — intra-zone scattering; 2 — inter-zone scattering. The experimental points are taken from [2]

$$K_{\beta\alpha 12}^{nm} = -\frac{2V}{(2\pi)^3} \frac{32\pi^6 e^4 \hbar^2 \gamma^{10}}{675 \varepsilon_0^2 a_0 \omega_0 k_B T} \times$$

$$\times \frac{M_{\text{Hg}} + M_{\text{Te}}}{M_{\text{Hg}} M_{\text{Te}}} \left(\frac{2m_{hh}}{\hbar^2} \right)^{3/2} \delta_{\alpha\beta} \int (N_{\vec{q}} + 1) f_0(\varepsilon) \times$$

$$\times [1 - f_0(\varepsilon - \hbar\omega_0)] (-\varepsilon - \varepsilon_g + \hbar\omega_0)^{1/2} k^4(\varepsilon) \times$$

$$\times \frac{\partial k(\varepsilon)}{\partial \varepsilon} \varepsilon^{n+m} d\varepsilon,$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol; $f_0(\varepsilon)$ is the Fermi—Dirac function; and $\theta(x)$ — the step function.

Calculation of the temperature dependence of electrons' mobility has been carried out with taking the acceptors' concentration to be equal $N_A = 10^{15} \text{ cm}^{-3}$; in so doing, we neglected the heavy holes'

contribution that constitutes approximately 1 %. In our calculation, we have taken into account the same scattering mechanisms as in work [3]. As is seen from Fig. 3, the theoretically predicted curve is in good agreement with the experimental data for $T > 100 \text{ K}$ thus confirming an adequacy of our model describing the scattering of electrons by polar optical phonons, in contrast with the model of work [1]. It is also seen from Fig. 3 that the intra-zone scattering by polar optical phonons is the main scattering mechanism at $T > 100 \text{ K}$. The contribution of inter-zone scattering under the above temperatures is minor and may be neglected.

Conclusion

A model of electrons' inelastic scattering by polar optical phonons in HgTe is developed. It provides a good agreement between the predicted and measured results within the frame of the exact solution of the Boltzmann stationary equation for temperatures above 100 K.

1. *Szymanska W., Dieltl T.* // J. Phys. Chem. Solids.—1978.—**39**.— P.1025—1040.
2. *Dubowski J., Dieltl T., Szymanska W.* // J. Phys. Chem. Solids.—1981.—**42**.— P.351—362.
3. *Matyk O.P.* // Ukr. Fiz. Zh. — 2002.— **47**, N 9. — P. 842—845.
4. *Bonch-Bruevich V.L., Kalashnikov S.G.* Physics of Semiconductors. — Moscow: Nauka, 1977 (in Russian).

Received 06.07.03

Translated from Ukrainian by A.G. Filin

НЕПРУЖНЕ РОЗСІЯННЯ ЕЛЕКТРОНІВ НА ПОЛЯРНИХ ОПТИЧНИХ ФОНОНАХ У ТЕЛУРИДІ РТУТІ

О. П. Малик

Резюме

Запропоновано модель непружного розсіяння електронів на полярних оптичних фононах, в якій імовірність розсіяння не залежить від макроскопічного параметра — діелектричної проникності кристала. Розглянута модель дає добре узгодження між теорією та експериментом в інтервалі температур 77—300 К.