ELSEVIER

Materials Science and Engineering B 129 (2006) 161–171

MATERIALS SCIENCE & ENGINEERING B

www.elsevier.com/locate/mseb

# Electron scattering on the short-range potential in narrow gap $Cd_xHg_{1-x}Te$

O.P. Malyk

*Lviv Polytechnic National University, Semiconductor Electronics Department, Bandera Street 12, 79013 Lviv, Ukraine*

Received 1 September 2005; received in revised form 31 October 2005; accepted 12 January 2006

**Abstract**

Models of electron scattering on the short-range potential caused by the interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, ionized and neutral impurities in the narrow gap solid solution $Cd_xHg_{1-x}Te$ ($x = 0$, 0.08, 0.17, 0.26 and 0.36) are proposed. The temperature dependences of electron mobility in temperature range 4.2–300 K are calculated.


*Keyword:* Theory of scattering

## 1. Introduction

The electron scattering in the solid solution $Cd_xHg_{1-x}Te$ was considered in relaxation time approximation in Ref. [1–3]. The models of electron scattering on the lattice defects used in these works have essential shortcoming—they are long-range which contradicts special relativity. Besides the use of a macroscopic parameter in these models, the permittivity is not reasonable in microscopic processes. From the other side in Refs. [4–6], the short-range model of electron–polar optical phonon scattering was proposed in which the above mentioned shortcomings were absent. Here the following physical reasons were used: during the scattering the electron interacts only with neighboring crystal region (the short-range principle), after the scattering on this region the electron interacts with the next neighboring crystal region, etc. As a neighboring region, the elementary cell (a structural unit of a crystal) gets out. The purpose of the present work is to use the approach advanced in these works for construction of the short-range scattering models on various types of crystal defects.

## 2. Short-range scattering models

### 2.1. Electron–polar optical phonon scattering

The expression for electron transition probability connected with polar optical phonon absorption and radiation looks like:

$$W(\mathbf{k},\mathbf{k}') = \frac{64\pi^7\gamma_{PO}^{10}e^4}{225\,\varepsilon_0{}^2a_0{}^4G}\,\frac{M_x+M_{Te}}{M_xM_{Te}}\left\{\frac{1}{\omega_{LO}}[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO})+(N_{LO}+1)\times\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})]\right.$$
$$\left.+\,\frac{2}{\omega_{TO}}[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO})+(N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})]\right\}, \quad (1)$$

where $M_x = xM_{Cd} + (1-x)M_{Hg}$, $M_{Cd}$, $M_{Te}$ is the atom masses; $G$ the number of unit cells in a crystal volume; $\varepsilon_0$ the dielectric constant; $e$ the elementary charge; $\alpha_0$ the lattice constant; $\gamma_{PO}$ the adjustable parameter determining the action radius of short-range

*E-mail address:* omalyk@mail.lviv.ua.

0921-5107/$ – see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.mseb.2006.01.007

potential ($R = \gamma_{PO}\,\alpha_0$) and $N_{LO}$; $N_{TO}$ are the number of longitudinal (LO) and transverse (TO) phonons with a frequency $\omega_{LO}$ and $\omega_{TO}$, respectively.

Expression (1) differs from that obtained in Refs. [4–6] by presence of the component which takes into account the electron interaction with transverse phonons. Using the formalism of a precise solution of the stationary Boltzmann equation [7,8] one can obtain the values $K_{\beta\alpha}^{nm}$ for this scattering mechanism:

$$K_{\beta\alpha}^{nm} = -\frac{2V}{(2\pi)^3}\frac{64\,\pi^6 e^4\hbar^2\gamma_{PO}^{10}\delta_{\alpha\beta}}{675\,\varepsilon_0{}^2 a_0\,k_B T}\frac{M_x + M_{Te}}{M_x M_{Te}}\left[\frac{1}{\omega_{LO}}\int\left\{N_{LO}\,f_0(\varepsilon)[1 - f_0(\varepsilon+\hbar\omega_{LO})]\times k^2(\varepsilon+\hbar\omega_{LO})\frac{\partial k(\varepsilon+\hbar\omega_{LO})}{\partial\varepsilon}\right.\right.$$
$$\left. + (N_{LO}+1)\,\theta(\varepsilon-\hbar\omega_{LO})\,f_0(\varepsilon)[1 - f_0(\varepsilon-\hbar\omega_{LO})]\times k^2(\varepsilon-\hbar\omega_{LO})\,\frac{\partial k(\varepsilon-\hbar\omega_{LO})}{\partial\varepsilon}\right\}$$
$$\times k^4(\varepsilon)\frac{\partial k(\varepsilon)}{\partial\varepsilon}\varepsilon^{n+m}\mathrm{d}\varepsilon + \frac{2}{\omega_{TO}}\int\left\{N_{TO}\,f_0(\varepsilon)[1 - f_0(\varepsilon+\hbar\omega_{TO})]\times k^2(\varepsilon+\hbar\omega_{TO})\frac{\partial k(\varepsilon+\hbar\omega_{TO})}{\partial\varepsilon}\right.$$
$$\left.\left. + (N_{TO}+1)\,\theta(\varepsilon-\hbar\omega_{TO})\,f_0(\varepsilon)[1 - f_0(\varepsilon-\hbar\omega_{TO})]k^2(\varepsilon-\hbar\omega_{TO})\times\,\frac{\partial k(\varepsilon-\hbar\omega_{TO})}{\partial\varepsilon}\right\}k^4(\varepsilon)\,\frac{\partial k(\varepsilon)}{\partial\varepsilon}\varepsilon^{n+m}\mathrm{d}\varepsilon\right], \tag{2}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta; $f_0(\varepsilon)$ the Fermi–Dirac function; $\theta(x)$ the step function and $k_B$ is the Boltzmann constant.

### 2.2. Electron–nonpolar optical phonon scattering

The potential energy caused by the electron–nonpolar optical phonon interaction looks like [9]:

$$U = \sum_{\mathbf{q}\,\nu}\left[\frac{\hbar}{2G\omega_\nu(\mathbf{q})}\frac{M_x + M_{Te}}{M_x M_{Te}}\right]^{1/2}\mathbf{Q}*\mathbf{W}^0(\mathbf{r})\left[b_{\mathbf{q},\nu}\mathrm{e}^{\mathrm{i}\,\mathbf{q}\boldsymbol{\rho}} + b_{\mathbf{q},\nu}^*\mathrm{e}^{-\mathrm{i}\,\mathbf{q}\boldsymbol{\rho}}\right], \tag{3}$$

where $\mathbf{W}^0(\mathbf{r})$ is the optical deformation potential with the periodicity of the crystal lattice; $\boldsymbol{Q}$ the unit vector of displacement of the atom; $\mathbf{q}$ and $\omega_\nu(\boldsymbol{q})$ the wave vector and angular frequency of the $\nu$th branch of optical oscillations in the crystal ($\nu = 4, 5, 6$); $b_{\mathbf{q},\nu}$ and $b_{\mathbf{q},\nu}^*$ are phonon annihilation and creation operators, respectively, of the $\nu$th branch with wave vector $\mathbf{q}$; $\boldsymbol{\rho} = \mathbf{i}(n_2+n_3)(a_0/2) + \mathbf{j}(n_1+n_3)(a_0/2) + \mathbf{k}(n_2+n_1)(a_0/2)$, ($n_1$, $n_2$, $n_3 = 1, 2, \ldots$), $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ are unit vectors along the principal crystal axes. Later on the change of coordinate will be considered only within the limits of one unit cell thus the potential (3) becomes short-range.

To calculate the transition probability connected with electron–phonon interaction, let us write the wave function of the electron–phonon system in the form:

$$\Psi = \frac{1}{\sqrt{V}}\exp(\mathrm{i}\,\mathbf{kr})\Phi(x_1, x_2, \ldots, x_n), \tag{4}$$

where $V$ is the crystal volume and $\Phi(x_1, x_2, \ldots, x_n)$ is the wave function of the system of independent harmonic oscillators.

Then a transition matrix element from interaction energy looks like:

$$\langle N'_{\mathbf{q}}, \mathbf{k}'|U|N_{\mathbf{q}}, \mathbf{k}\rangle$$
$$= \frac{1}{V}\sum_{\mathbf{q},\nu}\left[\frac{\hbar}{2G\omega_\nu(\mathbf{q})}\frac{M_x + M_{Te}}{M_x M_{Te}}\right]^{1/2}\int_\Omega \exp(\mathrm{i}\,\mathbf{sr})\mathbf{Q}*\mathbf{W}^0(\mathbf{r})\mathrm{d}\mathbf{r}$$
$$\times\int\Phi^*(x_1, x_2, \ldots, x_n)[b_{\mathbf{q}}\mathrm{e}^{\mathrm{i}\,\mathbf{q}\boldsymbol{\rho}} + b_{\mathbf{q}}^*\mathrm{e}^{-\mathrm{i}\,\mathbf{q}\boldsymbol{\rho}}]\Phi(x_1, x_2, \ldots, x_n)\mathrm{d}x_1\,\mathrm{d}x_2\,\ldots\,\mathrm{d}x_n,\ \Omega = \frac{a_0^3}{4},\ \mathbf{s} = \mathbf{k} - \mathbf{k}'. \tag{5}$$

Let us present the integral over the electron coordinates as:

$$\int_\Omega \exp(\mathrm{i}\,\mathbf{sr})\mathbf{Q}*\mathbf{W}^0(\mathbf{r})\mathrm{d}\mathbf{r} = \frac{a_0^2}{4}\frac{a_0}{\Omega}\int_\Omega \exp(\mathrm{i}\,\mathbf{sr})\mathbf{Q}*\mathbf{W}^0(\mathbf{r})\mathrm{d}\mathbf{r} = \frac{a_0^2}{4}d_0, \tag{6}$$

The integration over the harmonic oscillators coordinates gives the factors $\sqrt{N}$ and $\sqrt{N+1}$ ($N$ is the number of phonons with a corresponding frequency for one LO-mode ($\omega = \omega_{LO}$) and two TO-modes ($\omega = \omega_{TO}$)) for phonon annihilation and creation operators, respectively. To calculate the sum over the vector $\mathbf{q}$ let us make the following simplifications: (1) we take into consideration a quasicontinuous character of wave vector variation and pass from summation to integration over $\mathbf{q}$ and (2) we change from