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ELECTRON-PHONON SCATTERING IN QUANTUM-SIZED FILMS WITH THE HYPERBOLIC PÖSCHL–TELLER POTENTIAL

A quantitative theory of electron-phonon interaction in the two-dimensional electron gas in a quantum-sized film with the hyperbolic Pöschl–Teller confining potential has been developed. Analytical expressions for the transition probability are derived in the case of electron scattering by deformation-induced acoustic, piezoacoustic, and polar optical phonons. The results obtained for various scattering mechanisms in the film are compared with the results obtained for bulk crystals.

Keywords: quantum-sized film, electron-phonon interaction, hyperbolic potential, transition probability.

1. Introduction

Nowadays, one of the most rapidly developing scientific fields is the study of the physical and chemical properties of low-dimensional structures. Of particular practical interest are the electronic properties of nanostructures associated with quantum effects. In nanostructures, the free motion of electrons is confined, which results in a modification of the electron concentration character. The size quantization effect makes it possible to govern the physical properties of quantum-sized films and create devices with prescribed characteristics [1].

The processes of electron scattering by lattice vibrations in solids, phonons, substantially affect plenty of kinetic and optical phenomena. It is rather interesting to consider the features of electron scattering in low-dimensional structures, e.g., in quantum wells, where the size quantization effect has to be taken into consideration [2, 3].

Electron scattering by confined interface polar optical phonons in a double heterostructure was studied in works [4, 5]. The cited authors considered the rate of scattering of an electron in the quantum well by localized polar optical and interface phonons and showed that, by changing the semiconductor composition, the electron-phonon scattering rate can be varied. The electron-phonon interaction in InAs/AlS structures in the quantization magnetic field regime was studied in work [6].

Nanostructured ZnO thin films with various grain sizes were analyzed with the help of scanning electron microscopy, X-ray diffraction, and Raman spectroscopy. It was found that a decrease of the grain size is accompanied by a reduction of the electron-phonon coupling [7]. The dielectric parameters of TiO_2 thin films grown with the use of the radio-frequency magnetron sputtering method at various sputtering powers were studied in work [8]. In work [9], the experimental data obtained by scanning tunneling spectroscopy and the features of tunnel processes in semiconductor nanostructures were described and theoretically explained.

Earlier, we considered the problem of the screening of a scattering potential created by charge carriers in a quantum-sized thin film with the modified Pöschl–Teller potential [10]. In this work, we study the electron-phonon interaction with different scattering mechanisms in the same electron system.

2. Theory

While describing the physical processes in quantum nanostructures – in particular, in quantum wells (QWs) – the adequate mathematical modeling of a confining potential plays an important role. When a QW grows, there emerges a confining potential at the interface between the QW and the matrix (the environment). Therefore, the choice of the confining potential is very important. Potentials with rectangular or parabolic profiles are often used. However, the parabolic-like potential is realized only for lower energy levels, and its profile deviates from the parabola, as the quantum number increases. At the same time, if the energy of the particle increases, it feels the interface between the quantum well and the environment more and more strongly. As a result, there arises a necessity to consider the finite height of the confining potential on the one hand and the nonparabolic profile of the confining potential on the other hand. The indicated difficulties can be avoided by introducing more complicated and multiparametric potentials such as the Pöschl–Teller one. Therefore, in this work, in order to make the approximation of the generated confining potential more realistic, we propose to use the modified Pöschl–Teller potential [10, 11].

The determination of the transition probability is known to be a problem of quantum scattering theory. This problem is solved in the framework of the nonstationary perturbation theory [12]. The total Hamiltonian of an electron in a real lattice can be written in the form [13, 14]

$$\hat{H}_e = \hat{H} + \hat{H}'. \tag{1}$$

Here, the term $\hat{H}'$ describes the interaction of the electron with phonons, which is considered to be a small perturbation to the unperturbed Hamiltonian $\hat{H}$. The latter, in the case of phonon scattering, also includes the Hamiltonian of an ideal phonon gas that does not interact with the electron. Since a unit cell remains almost undeformed at long-wave acoustic vibrations (only its center of mass oscillates), the interaction energy cannot be proportional to the cell displacement itself. Instead, it has to be a linear function of the first derivatives of the cell displacement $\mathbf{u}_{\rm ac}(\mathbf{r})$ along the coordinates:

$$\hat{H}'_{\rm ac} = E_1 \operatorname{div} \mathbf{u}_{\rm ac}(\mathbf{r}), \tag{2}$$

where $\mathbf{r}$ is the vector corresponding to the cell position. This function is called the deformation potential, and the proportionality coefficient E_1 is the deformation potential constant. Then, according to works [13, 14], we may write

$$\mathbf{u}_{\rm ac}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{j=1}^{3} \mathbf{e}_i(\mathbf{q}) \times \\ \times \left[b_j(\mathbf{q}) e^{i\mathbf{qr}} + b_j^*(\mathbf{q}) e^{-i\mathbf{qr}} \right], \tag{3}$$

where $\mathbf{e}_i(\mathbf{q})$ is the unit polarization vector, $b_j(\mathbf{q})$ $(j = 1, 2, 3)$ are the complex normal coordinates, and N is the number of unit cells that determine lattice vibrations.

Substituting (3) into (2), we obtain

$$\hat{H}'_{\rm ac}(r) = \frac{iE_1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{j=1}^{3} (\mathbf{q}\mathbf{e}_i(\mathbf{q})) \times \\ \times \left[b_j(\mathbf{q}) e^{i\mathbf{qr}} + b_j^*(\mathbf{q}) e^{-i\mathbf{qr}} \right]. \tag{4}$$

Let the wave function of the system "electron + + phonon" be represented in the form $|\beta N_{\mathbf{q}j}\rangle$, where β is a set of quantum numbers that characterize the electron state. In our case, $\beta = (\lambda, n, \mathbf{k}_{\rm 2D}, \sigma)$, where $\mathbf{k}_{\rm 2D}$ is the two-dimensional wave vector, and σ is the spin quantum number. The parameter $N_{\mathbf{q}j}$ characterizes the number of phonons with the wave vector $\mathbf{q}$ and the polarization j.

Let us calculate the scattering probability for the hyperbolic Pöschl–Teller potential. The latter looks like [10, 11]

$$V(z) = \frac{\hbar^2\alpha^2}{2m} \lambda(\lambda+1) \tanh^2 \alpha z, \tag{5}$$

where α and λ are the parameters of the potential well, which characterize its depth and half-width, respectively. For an electron in the thin film with potential (5), its motion is quantized in the z-direction (perpendicularly to the film), but it remains classical in the film plane (x, y). Accordingly, the total electron energy

$$\varepsilon = \frac{\hbar^2\alpha^2}{2m} \left(\lambda(\lambda+1) - (\lambda - n)^2 \right) + \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} \tag{6}$$

consists of a discrete component and a continuous one, with the latter being typical of bulk crystals.

Hence, the electron energy spectra in thin films is a set of size-quantized subbands. Within every subband, the energy varies in a quasicontinuous manner. The electron wave functions in those subbands can be written as follows:

$$\psi_{n,k_x,k_y,\lambda}(x,y,z) = \\ = e^{i(k_x x+k_y y)}\left(\frac{\alpha(\lambda-n)\Gamma(2\lambda n+1)}{\Gamma(n+1)}\right)^{1/2}\times \\ \times L_n^z(\lambda,\ n-\lambda,\tanh\alpha z). \quad (7)$$

Here, the integer number n varies from 0 to a positive integer number λ, k_x and k_y are the projections of the electron wave vector onto the film plane, and $L_n^z(x)$ is the Legendre function. In this case, the calculation of the $H'_{\rm ac}$-matrix element between the phonon functions brings us to the formula [13, 14]

$$\left\langle N'_{\mathbf{q}j}\left|H'_{\rm ac}\right|N_{\mathbf{q}j}\right\rangle = \sqrt{\frac{\hbar\left(N_{\mathbf{q}j}+\frac{1}{2}\mp\frac{1}{2}\right)}{2M\omega_j(\mathbf{q})}}\ \delta_{N'_{\mathbf{q}j},N_{\mathbf{q}j}\mp1}. \quad (8)$$

At the same time, the calculation of the factor $e^{iq_z z}$ between the electron wave functions with potential [5] gives

$$\left\langle\lambda',n',\mathbf{k}'_{2\rm D},\sigma'\right|e^{iq_z z}\left|\lambda,n,\mathbf{k}_{2\rm D},\sigma\right\rangle = \\ = \left\langle\lambda',n'\left|e^{iq_z z}\right|\lambda,n\right\rangle\ \delta_{\sigma',\sigma}\delta_{\mathbf{k}'_{2\rm D},\mathbf{k}_{2\rm D}\pm\mathbf{q}_{2\rm D}}. \quad (9)$$

For the values $\lambda=\lambda'=1$ and $n=n'=0$, this matrix element equals

$$\left\langle\lambda'=1,n'=0\right|\left.e^{iq_z z}\right|\lambda=1,n=0\right\rangle = \\ = \frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}. \quad (10)$$

Then the scattering probability looks like [2]

$$W = \frac{2\pi}{\hbar}\sum_{N_{qj}}\frac{\hbar\left(N_{\mathbf{q}j}+\frac{1}{2}\mp\frac{1}{2}\right)}{2NM\omega_j(\mathbf{q})}(E_1 q)^2\times \\ \times\left(\frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2\delta_{N'_{\mathbf{q}j},N_{\mathbf{q}j}\mp1}. \quad (11)$$

Using formulas (11.34) and (11.35) from work [13], we obtain

$$W_{\rm ac} = \sum_q w_1(\mathbf{q})\left(A^+ + A^-\right), \quad (12)$$

where

$$A^{\pm} = \left(N_{\mathbf{q}}+\frac{1}{2}\mp\frac{1}{2}\right)\delta\left(\varepsilon_{\beta,\mathbf{k}'_{2\rm D}}-\varepsilon_{\beta,\mathbf{k}_{2\rm D}}\mp\hbar\omega(\mathbf{q})\right)\times \\ \times\delta_{\sigma',\sigma}\delta_{\mathbf{k}'_{2\rm D},\mathbf{k}_{2\rm D}\pm\mathbf{q}_{2\rm D}}, \quad (13)$$

$$w_1(\mathbf{q}) = \frac{\pi(E_1 q)}{N}M\omega(\mathbf{q})^2\left(\frac{\pi q_z\ \mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2. \quad (14)$$

Here, we assumed that electrons occupy the lower subband ($\lambda=1, n=0$), and the spin degeneracy is neglected. A further simplification is obtained, if we assume the scattering to be elastic at $k_{\rm B}T>\hbar\omega(q)$. Then

$$W = \frac{2\pi E_1^2 k_{\rm B}T}{NM\hbar V_o^2}\left(\frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2\delta\left(\varepsilon_{\beta,\mathbf{k}'_{2\rm D}}-\varepsilon_{\beta,\mathbf{k}_{2\rm D}}\right).$$

If the inverse relaxation time and the screening are also taken into account, the final expression for the transition probability at the deformation-acoustic phonon scattering reads

$$W^{\pm}(\mathbf{k}'_{2\rm D},\mathbf{k}_{2\rm D}) = \frac{2\pi}{\hbar}\sum_{\mathbf{q},\sigma'}\frac{\pi(E_1 q)^2}{2NM\omega(\mathbf{q})}\times \\ \times\left(N_{\mathbf{q}}+\frac{1}{2}\pm\frac{1}{2}\right)\left(\frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2\times \\ \times\delta_{\sigma',\sigma}\delta_{\mathbf{k}'_{2\rm D},\mathbf{k}_{2\rm D}\pm\mathbf{q}_{2\rm D}}\delta\left(\varepsilon_{\beta,\mathbf{k}'_{2\rm D}}-\varepsilon_{\beta,\mathbf{k}_{2\rm D}}\mp\hbar\omega(\mathbf{q})\right). \quad (15)$$

Expression (15) describes the scattering of electrons by acoustic phonons with potential (5).

The scattering by acoustic lattice vibrations occurs in every crystal irrespective of its unit cell complexity. If a crystal has a simple lattice (one atom per unit cell), the scattering by acoustic vibrations is the only mechanism of lattice interaction with charge carriers. In crystals with two or more atoms or ions per unit cell, besides the scattering by acoustic vibrations, the screening by optical and piezoelectric lattice vibrations has to be taken into account. If there is no symmetry center in crystals, and if some bonds have an ionic character, the propagation of acoustic waves results not only in the appearance of a deformation potential. In addition, a potential of the electrical origin, a piezoelectric potential, may also arise. This gives rise to the electron screening by piezoelectric phonons in those crystals. In this case,

the corresponding expression for the transition probability, which takes potential (5) into account, looks like

$$W^{\pm}\left(\mathbf{k}'_{2\mathrm{D}},\mathbf{k}_{2\mathrm{D}}\right)=\frac{2\pi}{\hbar}\sum_{\mathbf{q},\sigma'}\frac{\pi\left(E_{pz}q\right)^2}{2N\chi^2M\omega\left(\mathbf{q}\right)}\times$$
$$\times\left(N_{\mathbf{q}}+\frac{1}{2}\pm\frac{1}{2}\right)\left(\frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2\times$$
$$\times\delta_{\sigma',\sigma}\delta_{\mathbf{k}'_{2\mathrm{D}},\mathbf{k}_{2\mathrm{D}}\pm\mathbf{q}_{2\mathrm{D}}}\delta\left(\varepsilon_{\beta,\mathbf{k}'_{2\mathrm{D}}}-\varepsilon_{\beta,\mathbf{k}_{2\mathrm{D}}}\mp\hbar\omega\left(\mathbf{q}\right)\right).\quad(16)$$

In crystals with covalent bonds – i.e. in heteropolar ionic semiconductors – electrons are also scattered by polar optical phonons. Making allowance for this scattering with potential (5), we obtain

$$W^{\pm}\left(\mathbf{k}'_{2\mathrm{D}},\mathbf{k}_{2\mathrm{D}}\right)=\frac{2\pi}{\hbar}\sum_{\mathbf{q},\sigma'}\frac{4\pi e^2}{2N\chi^{*2}M\omega_0q^2}\times$$
$$\times\left(N_0+\frac{1}{2}\pm\frac{1}{2}\right)\left(\frac{\pi q_z\,\mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2\times$$
$$\times\delta_{\sigma',\sigma}\delta_{\mathbf{k}'_{2\mathrm{D}},\mathbf{k}_{2\mathrm{D}}\pm\mathbf{q}_{2\mathrm{D}}}\delta\left(\varepsilon_{\beta,\mathbf{k}'_{2\mathrm{D}}}-\varepsilon_{\beta,\mathbf{k}_{2\mathrm{D}}}\mp\hbar\omega\left(\mathbf{q}\right)\right).\quad(17)$$

One can see that, in all expressions (15)–(17) that describe the electron-phonon scattering in a quantum well with potential (5), there arises a factor $\left(\frac{\pi q_z\ \mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2$ in comparison with the case of bulk specimen [2].

3. Conclusions

In this paper, the expressions for the electron transition probability in the case of various scattering mechanisms in a quantum-sized thin film with the modified Pöschl–Teller potential have been obtained. It is shown that those expressions differ from their counterparts obtained for the electron screening in bulk crystals by the factor $\left(\frac{\pi q_z\ \mathrm{cosech}\,\frac{\pi q_z}{2\alpha}}{2\alpha}\right)^2$.

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ЕЛЕКТРОН-ФОНОННЕ РОЗСІЯННЯ КВАНТОВО-РОЗМІРНОЇ ПЛІВКИ З ГІПЕРБОЛІЧНИМ ПОТЕНЦІАЛОМ ПЕШЛЯ–ТЕЛЛЕРА

Р е з ю м е

Розвинена кількісна теорія електрон-фононної взаємодії для двовимірного електронного газу в квантовій плівці з гіперболічним утримуючим потенціалом Пешля–Теллера. Отримано аналітичні вирази ймовірності переходу при розсіянні електронів на деформаційно-акустичних, п'єзоакустичних і полярних оптичних фононах. Отримані результати для різних механізмів розсіювання порівнювалися з об'ємними кристалами.