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Control over Electron-Phonon Interaction Parameters in Quantum Wells by Changing Barrier Dielectric Properties

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***Abstract*—Influence of the barrier dielectric properties on the electron-phonon interaction in quantum wells is studied theoretically. It is shown that the parameters of such interaction can change several times. This leads to a similar change in the binding energy and the radius of polaron states arising in the structure. An increase in the electron-phonon interaction is confirmed to be possible in both symmetric and asymmetric quantum wells. It is found under which conditions the electron-phonon interaction in the asymmetric quantum well changes more strongly than in the symmetric one. This makes it possible to efficiently control over the parameters of polaron states by choosing the dielectric properties and symmetry of the barriers.**

Keywords—quantum well; dielectric properties; phonon engineering; interface phonons; polaron

I. INTRODUCTION

Modern technologies give us the possibility to effectively change the phonon properties of semiconductor nanostructures. Phonon states engineering now is applied to a wide range of practical uses [1,2]. The most interesting in this regard is the modification of electrical, optical and thermal properties of nanostructures [3,4].

Special attention should be paid to parameters of the electron-phonon interaction. These parameters can change significantly in quantum nanostructures compared with bulk materials. Our interest is the interaction of charged particles with polar optical phonons. The strong electron-phonon interaction can be realized in symmetric quantum wells when the large-radius polarons arise [5].

In this paper, the charged particle interaction with optical phonons have been studied theoretically and a comparative analysis for quantum wells with symmetric and asymmetric barriers is performed. The structures under study contain quantum wells with the barriers made of materials with different dielectric properties. Most researches focus on the electronic properties of such structures. But such quantum wells may also have specific optical phonon spectrum properties. In our work, is studied three-layered structure consisting of the quantum well and two barriers. It was found that in structures with asymmetric barriers the electron-phonon interaction can be stronger than with symmetric barriers one. This occurs because several branches of optical phonon spectrum of asymmetric structures give a comparable contribution to the electron-phonon interaction. In the case of symmetric case, as a rule, only one phonon mode gives the main influence.

II. SYMMETRIC QUANTUM WELL

To consider the interaction of charged particles with optical phonons of the quantum well and the barriers, as well as the interface phonons must be taken into account. Start with the case of complete localization of charged particles within a quantum well. Wherein the interaction of such particles with barrier material phonons can be neglected. However the influence of the barriers is very important. This effect is conditioned by the specific structure and properties of interface optical phonon spectrum. To define the properties of interface phonons, we use the continuum model from [6]. The spectrum of the symmetric mode of interface phonons is obtained from the solution of this equation:

$$\varepsilon^{w}(\omega) th\left(\frac{qL}{2}\right)+\varepsilon^{b}(\omega)=0 \qquad (1)$$

Here l is the quantum well characteristic size, q is two-dimensional wave vector; $\varepsilon^{w}(\omega)$, $\varepsilon^{b}(\omega)$ are the dielectric functions of the quantum well and barriers, respectively. The dependencies frequency of the dielectric function in the phonon frequency region is determined as follows:

$$\varepsilon(\omega)=\varepsilon_{\infty}\frac{\omega^2-\omega_{LO}^2}{\omega^2-\omega_{TO}^2}, \qquad (2)$$

where ω_{LO} , ω_{TO} are the frequencies of longitudinal and transverse optical phonons, respectively and ε_{∞} is the high-frequency dielectric constant. The equation (2) shows that we use the approximation of dispersion less modes for bulk optical phonons. In such approximation the interface and bulk phonon modes can be considered independently [1]. The contribution of the antisymmetric mode of interface phonons vanishes when the Hamiltonian is averaged over the

wave function of the charged particle localized in a symmetric quantum well. We have taken the case of the electron polaron. The magnification of the electron-phonon interaction occurs in narrow quantum wells having a width l that is less than the polaron radius r_0:

$$l < r_0 . \quad (3)$$

If the condition (3) is satisfied, the electron wave function $\Phi_m^{(e)}(\mathbf{r})$ can be written as:

$$\Phi_n^{(e)}(\mathbf{r}) = \psi_n(z)\chi_n(\boldsymbol{\rho}), \quad (4)$$

Where z is the transvers plane well variable, $\psi_n(z)$ is the wave function determined by the quantum well potential, $\boldsymbol{\rho}$ is the two–dimensional plane well vector, $\chi_n(\boldsymbol{\rho})$ is yet unknown two-dimensional wave function which is determined by localization of an electron in the potential well created by polar optical phonons.

Using the expression for the wave function from (4) and solving the problem by minimizing the functional that we obtained in [7] the polaron binding energy E_p is written in the form:,

$$\mathrm{E}_p = -0.4\frac{m\,e^4}{\left(\varepsilon_{opt}^b \hbar\right)^2}, \quad (5)$$

where ε_{opt}^b is the barrier optical dielectric function which is defined by the expression $\frac{1}{\varepsilon_{opt}^b} = \frac{1}{\varepsilon_\infty^b} - \frac{1}{\varepsilon_0^b}$.

Taken into account (5) one can obtain the polaron state radius r_0 in the form:

$$r_0 = \frac{\hbar^2 \varepsilon_{opt}^b}{m\,e^2}. \quad (6)$$

It is this quantity from (3) on which the adiabatic approximation used in our work is based. In the next order in the parameter from inequality (3) the corrections to (5) can be calculated. We can write its as follows:

$$\Delta\mathrm{E}_{pol,well} = 0.07\mathrm{E}_p \frac{l}{r_0}\left(D_V + D_S\right), \quad (7)$$

where the dimensionless coefficients D_V and D_S are determined by phonon frequencies combinations in the quantum well and barrier materials and are found similar to [7]. It should be noted that the corrections to the polaron binding energy are related to the interaction with both bulk and interface optical phonons. According to the expressions for D_V and D_S received in [7], these corrections may have different signs. Thus it turns out that the total value of the binding energy depends essentially on the dielectric properties of both the quantum well and the barrier materials. To calculate numerically the value of the quantity $\Delta\mathrm{E}_p$ from (7) one has taking into consideration the phonon spectrum of the structure.

In quantum wells based on II-VI compounds, the polaron radius r_0 (6) falls within the range $20 \div 100$ Å. Just than the strong electron-phonon interaction condition can be satisfied. Hence, the quasi-two-dimensional polaron state is possible in sufficiently narrow quantum wells with $l < 20$ Å.

The heterovalent quantum wells based on II-VI/III-V materials are more promising target for the experimental study of polaron effects in the case of strong electron-phonon interaction. For such structures, growth technologies have been developing successfully in recent times [8,9]. In the III-V compounds, effective masses of quantum well carriers are small. The optical dielectric function of the barriers fabricated from II-VI compounds is significantly small and values of polaron radius r_0 increase by two-three times. Hence, a quasi-two-dimensional polaron in heterovalent quantum wells can be observed for the well widths $L \le 50$ Å. Quantum wells of more complex configuration (for example, I-VII/III-V) can also become a promising object for the polaron study when strong electron-phonon interaction takes place.

III. Quantum Well with Asymmetric Barriers

We consider three-layered planar structure composed of a quantum well having a dielectric function $\varepsilon_w(\omega)$ and two different barriers with the dielectric functions $\varepsilon_{left}(\omega)$ and $\varepsilon_{right}(\omega)$. The dielectric functions of the left and right barriers are denoted by subscripts *l* and *r*, respectively. In the region of phonon frequencies, all dielectric functions have the form similar to expression (2):

$$\varepsilon^k(\omega) = \varepsilon_\infty^k \frac{\left(\omega_{LO}^k\right)^2 - \omega^2}{\left(\omega_{TO}^k\right)^2 - \omega^2}, \quad (8)$$

where ω_{LO}^k is longitudinal phonon frequency and ω_{TO}^k is transverse phonon one. The index k corresponds to “left” (*l*), “right” (*r*) for the barrier materials and “well” (*w*) for the quantum well material. The interface optical phonons will be of the most interest for our study. Their spectrum can be determined using standard conditions at two boundaries of the quantum well [6]. For the structure under consideration, it is found by solving the following equation:

$$e^{-|\mathbf{q}|l}\frac{\varepsilon^w(\omega) - \varepsilon^l(\omega)}{\varepsilon^w(\omega) + \varepsilon^l(\omega)} = e^{|\mathbf{q}|l}\frac{\varepsilon^w(\omega) + \varepsilon^r(\omega)}{\varepsilon^w(\omega) - \varepsilon^r(\omega)}, \quad (9)$$

where $\mathbf{q}$ is two-dimensional phonon wave vector in the well plane. Usually the solution of (9) corresponds to two branches of optical phonons localized near the left boundary of a quantum well and also two branches localized near the right one. These branches interact with each other that leads to a rather complicated picture for the electron-phonon interaction. The spectrum of optical phonons and the electron-phonon interaction nature are considerably

simplified for narrow quantum wells. Generally, the interaction in the region of polaron state radius r_0 is of the greatest interest. It corresponds to the values of the wave vector $q \approx r_0^{-1}$. The condition

$$ql \gg 1 \qquad (10)$$

is usually realized in semiconductor wells with the width of $l \gg 50$ Å. The equation (9) becomes much easier. In the highest order in parameter (10), the dielectric properties of the quantum well material completely drop out of the (9). Thus, we can obtain from (3) the following equation:

$$\varepsilon^r(\omega) + \varepsilon^l(\omega) = 0. \qquad (11)$$

Equation (11) formally coincides with the equation for determining the spectrum of interface phonons at a single hetero-interface [6]. In the presence of asymmetric barriers with $\varepsilon^r(\omega) \neq \varepsilon^l(\omega)$, it has two solutions for the interface phonons. Exact equation (9) contains two other spectrum branches that drop out of approximate equation (11). The solutions corresponding to (11) ω_1 and ω_2 are found to be in the following frequency intervals:

$$\begin{aligned} &\omega_{TO}^l < \omega_1 < \omega_{LO}^l \\ &\omega_{TO}^r < \omega_2 < \omega_{LO}^r \end{aligned}. \qquad (12)$$

Applying the method used in [6] we can obtain the Hamiltonian of the electron-phonon interaction $H_{el-phon}$ for the quantum well. It can be represented in the same form as in the case of a symmetric structure [10]

$$H_{el-phon,i} = \sum_{\mathbf{q}} \left(\frac{2\pi\omega_i e^2}{2S} \right)^{1/2} \frac{\exp(i\mathbf{q}\boldsymbol{\rho})}{\sqrt{2q}} f_i(\mathbf{q}, z) \cdot \cdot F_i(q, \omega_i) \left(a_i(\mathbf{q}) + a_i^+(\mathbf{q}) \right) \qquad (13)$$

In this equation i is the frequency interval number, S is the quantum well normalization area, $a_i(\mathbf{q})$ and $a_i^+(\mathbf{q})$ are the annihilation and creation operators of corresponding optical phonon branch. There are 4 branches in the full spectrum and 2 ones in the region $ql \gg 1$. The factor $f_i(\mathbf{q}, z)$ represents the distribution of the excitation intensity along the direction perpendicular to the quantum well plane. In the case under consideration, inside the quantum well at $|z| \leq l/2$, it has the form:

$$f_i(\mathbf{q}, z) = \gamma_i(\omega_i) e^{qz} + \gamma_i^{-1}(\omega_i) e^{-qz}, \qquad (14)$$

where the parameter $\gamma_i(\omega_i)$ is defined by the following expression:

$$\gamma_i(\omega_i) = e^{-ql} \frac{\varepsilon^w(\omega_i) + \varepsilon^l(\omega_i)}{\varepsilon^w(\omega_i) - \varepsilon^l(\omega_i)} = e^{qa} \frac{\varepsilon^w(\omega_i) + \varepsilon^r(\omega_i)}{\varepsilon^w(\omega_i) - \varepsilon^r(\omega_i)}. \qquad (15)$$

Equation (14) for $f_i(\mathbf{q}, z)$ differs from analogous expressions for the structures with symmetric barriers in that it is impossible to distinguish symmetric and antisymmetric modes. The greatest difference from quantum well with symmetric barriers can be found for the coefficients $F_i(q, \omega_i)$ which can be written through the quantities $R_{as}(\omega_i)$ as

$$R_{as} = \left| F_i(q, \omega_i) f_i(\mathbf{q}, z) \right|^2 = \frac{2\beta^r(\omega_i)\beta^l(\omega_i)}{\beta^r(\omega_i) + \beta^l(\omega_i)}, \qquad (16)$$

where the functions $\beta_i(\omega_i)$ have the form [6]:

$$\beta_i(\omega) = \left[\frac{1}{\varepsilon_{i,\infty}} - \frac{1}{\varepsilon_{i,0}} \right] \frac{\omega_{LO,i}^2}{\omega^2} \left[\frac{\omega^2 - \omega_{TO,i}^2}{\omega_{LO,i}^2 - \omega_{TO,i}^2} \right]^2 \qquad (17)$$

The results of our numerical calculations of the parameters R_{as} for various dielectric properties of the barriers are shown in Fig. 1 and Fig. 2. These dependencies are depicted for the different ratios of dielectric constants. Expression (16) means that in sufficiently narrow quantum wells the energy of the electron-phonon interaction can be represented as a constant over the well width. This value corresponds to the polarization created by the barriers. In sufficiently narrow quantum wells, this polarization varies slightly over the quantum well width. The dielectric properties of the quantum well material in this approximation turn out to be insignificant. The expression for the parameter R_{as} should be compared with the analogous expression for R_{sym}, which can be written when the constant of the electron-phonon interaction in symmetric quantum wells is found. Earlier it was shown in [5] that for symmetric structures, under condition (3), this value turns out to be equal to

$$R_{sim} = \frac{1}{\varepsilon_{opt}} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}, \qquad (18)$$

where the dielectric constats ε_∞ and ε_0 refer to the barriers. It is this quantity from the expression (5) for the polaron binding energy. Thus, the frequency of the interface mode is close to the frequency of longitudinal optical phonons ω_{LO} of the barrier material. The expressions for R_{sim} should correspond to the well where either the right (*r*) or left (*l*) barrier of an asymmetric structure is used for both barriers. In the case of the asymmetric structure with different barriers, the phonon frequency will slightly differ from both $\omega_{LO,l}$ and $\omega_{LO,r}$. It is important to take this difference into account in order to find correctly the

parameters of the electron-phonon interaction.

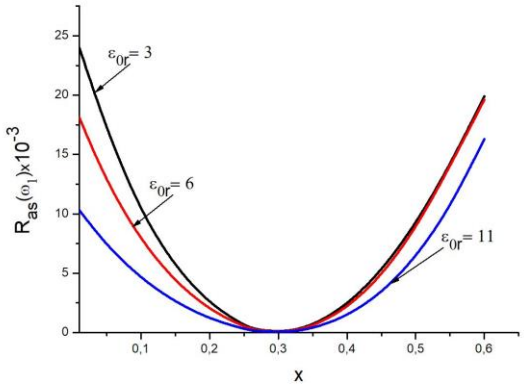

Fig. 1. *Coefficients* $R_{as}(\omega_1)$ *for the interface phonon frequencies* ω_1 *from the interval* $\omega_{TO}^{l} < \omega_1 < \omega_{LO}^{l}$.

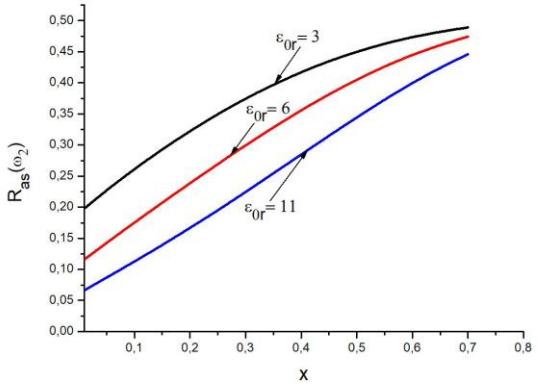

Fig. 2. *Coefficients* $R_{as}(\omega_2)$ *for the interface phonon frequencies* ω_1 *from the interval* $\omega_{TO}^{r} < \omega_2 < \omega_{LO}^{r}$.

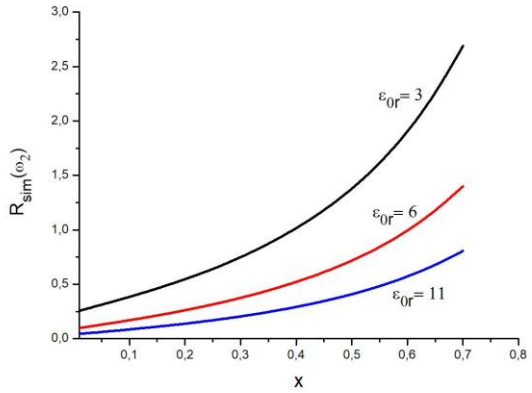

Fig. 3. *Coefficients* $R_{sim}(\omega_2)$ *for the interface phonon frequencies* ω_2 *from the interval* $\omega_{TO} < \omega_2 < \omega_{LO}$.

For comparison, similar dependencies Fig. 3 for R_{sim} are calculated for quantum wells with symmetric by their dielectric properties barriers. The varying quantity x in Fig. 1 – Fig. 3 describes the change in the frequency ratio for the longitudinal and transverse optical phonons.

IV. Results and Discussions

The interface optical phonons arise near the hetero-interface of the quantum well structure. The spectrum and dispersion law of such phonons may differ from ones for excitations arising in the bulk materials. The study of these excitations can give fundamentally new information about the optical and transport properties of quantum nanostructures. The theoretical method has been developed to taking into account the interface phonon influence. The enhancement conditions for electron-phonon interaction are found. It is shown that the barrier material dielectric properties give a decisive contribution to the polaron binding energy value for strong electron-phonon interaction. The appearance of strong polaron effects confirms the interface phonon influence on optical and transport properties of nanostructures. It was found that the strongest interaction is realized when the barriers in the quantum well structure are fabricated from materials with different dielectric properties for the left and right barriers. At a significant difference in the phonon frequencies of the barrier materials, the coupling constant value can exceed the analogous one for the quantum wells with symmetric barriers. Changing the parameters of the barriers makes it possible to change the value of the electron-phonon interaction constant by several times. This gives us the instrument for the control of nanostructure characteristics that determines many of the thermal, electrical, and optical properties.

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