Multiple changes in the electron-phonon interaction in quantum wells with dielectrically different barriers

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The specific features of the interaction of charged particles with polar optical phonons have been studied theoretically for quantum wells with the barriers that are asymmetric in their dielectric properties. It is shown that the interaction with interface phonon modes makes the greatest contribution in narrow quantum wells. The parameters of the electron-phonon interaction were found for the cases of different values of the phonon frequencies in the barrier materials. It turned out that a significant (by almost an order of magnitude) change in the parameters of the electron-phonon interaction can occur in such structures. This makes it possible, in principle, to trace the transition from weak to strong interactions in quantum wells of the same type but with different compositions of barrier materials. The conditions are found under which an enhancement of the electron-phonon interaction is possible in an asymmetric structure in comparison with a symmetric one with the barriers of the same composition.

Keywords: quantum well, electron-phonon interaction, polaron, asymmetric barriers.

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1. Introduction

Modern technology of semiconductor nanostructures manufacturing allows to efficiently change the phonon properties of such objects. Therefore, the term „phonon states engineering“ is widely used lately [1,2]. Spectrum of phonon states is critical for thermal properties of nanostructures and very important for modification of electrical and optical properties.

In nanostructures the electron-phonon interaction parameters also significantly change. Interaction of charged particles with polar optical phonons is of special interest. According to evaluations, the implementation of strong electron-phonon interaction with generation of large-radius polarons is possible in symmetric quantum wells [3]. For that purpose the use of quantum wells with barriers, made of materials with high level of ionicity, is required. At the same time, the ionicity of the quantum well material is not important. As far as we know, such excitations have not been experimentally observed yet. Significant change of electron-phonon interaction nature can be expected in quantum wells with barriers, asymmetric in terms of their dielectric properties. Such structures are studied experimentally lately [4–6]. Also they can be included as components in multi-layer structures, that are used for creation of solar cells [7–11]. Change of electron-phonon interaction nature is related to the fact, that in asymmetric structures several phonon spectrum branches should make the comparable contribution to the interaction. In case of symmetric structures only one phonon mode usually makes the prevailing contribution.

In this work we studied the specific features of the charged particles interaction with optical phonons for the quantum wells with barriers, asymmetric in terms of their dielectric properties. Model of dielectric continuum is used for phonon spectrum detection and electron-phonon interaction features determination. This approach allows to properly define the phonon properties of heterostructures in cases, when all characteristic parameters of the task with length size define the constant of a lattice of the materials in use. For structures, containing monoatomic layers, more complicated and lengthy theoretical models can be required. Under our approach it is shown that by means of barrier properties change the value of electron-phonon interaction can be changed by several times. The conditions are found, under which in asymmetric structure the enhancement of interaction compared to symmetric structure with the same barrier materials use can be implemented.

2. Interface phonons spectrum

Let's examine the three-layer planar structure, consisting of quantum well region with dielectric permittivity $\varepsilon_w(\omega)$ and two different barriers with permittivity $\varepsilon_l(\omega)$ and $\varepsilon_r(\omega)$. l and r indices indicate dielectric permittivity of the left and right barriers, respectively. In the area of phonon frequencies all dielectric functions are of the same kind:

$$\varepsilon_k(\omega) = \varepsilon_{\infty,k} \frac{\omega_{LO,k}^2 - \omega^2}{\omega_{TO,k}^2 - \omega^2} \qquad (1)$$

with different values of frequencies of longitudinal $\omega_{LO,k}$ and transversal $\omega_{TO,k}$ phonons. The index k here corresponds to l, r or w. With dielectric permittivity, defined with expression (1), the Lyddane–Sachs–Teller relation is applied

for all layers:

$$\varepsilon_k(0) = \varepsilon_{\infty,k} \frac{\omega_{LO,k}^2}{\omega_{TO,k}^2}. \quad (2)$$

Electronic spectrum of barriers is not significant for us. When examining the various barriers the significant is only the fact that in all cases they should result in localization of carriers in quantum well area. Interface optical phonons will be the most interesting object for us. Their spectrum can be found, using standard boundary conditions at two quantum well boundaries [12]. For the examined structure it is defined with the solving of the following equation:

$$e^{-|\mathbf{q}|a} \frac{\varepsilon_w(\omega) - \varepsilon_l(\omega)}{\varepsilon_w(\omega) + \varepsilon_l(\omega)} = e^{|\mathbf{q}|a} \frac{\varepsilon_w(\omega) + \varepsilon_r(\omega)}{\varepsilon_w(\omega) - \varepsilon_r(\omega)}. \quad (3)$$

Here, a is the quantum well width, $\mathbf{q}$ is the two-dimensional phonon vector in the well plane. In general case the solution of the equation (3) contains two branches of optical phonons, localized near the left boundary of the quantum well, and two branches of phonons, localized near the right boundary. These branches interact with each other, resulting in rather complicated picture for electron-phonon interaction.

Optical phonons spectrum and nature of electron-phonon interaction is significantly simplified for narrow quantum wells. Usually the interaction in the area with a size of about polar state radius r_p, that corresponds to the values of wave vector $q \approx r_p^{-1}$, is of the most interest. In case of meeting the condition

$$qa \ll 1. \quad (4)$$

that is usually implemented in semiconductor wells with a width of $L \sim 50$ Å, the equation (3) is significantly simplified. In high order as per parameter (4) the dielectric properties of the quantum well area completely fall out of it. As a result from (3) we get

$$\varepsilon_r(\omega) + \varepsilon_l(\omega) = 0. \quad (5)$$

Equation (5) formally corresponds with the equation for determination of interface phonons spectrum at a single heteroboundary [12]. In case of asymmetric barriers with $\varepsilon_r(\omega) \neq \varepsilon_l(\omega)$ it has two solutions for interface phonons. At the same time, for our three-layer structure one solution has the maximum intensity at the left well boundary, while another — at the right.

Two other branches, that contain the exact equation (3), fall out of the approximate equation (5). Areas of existence of equation (5) solutions depend on phonon spectra of barrier materials. If areas of phonon frequencies of the left and right boundaries materials overlap, the order of these frequencies location becomes important. Let's for definiteness assume that $\omega_{LO,l} < \omega_{LO,r}$, and $\omega_{TO,l} > \omega_{TO,r}$. Then the interface phonons frequencies appear in the following intervals:

$$\omega_{TO,r} < \omega_1 < \omega_{TO,l}$$

$$\omega_{LO,l} < \omega_2 < \omega_{LO,r}. \quad (6)$$

In case of change of phonons frequencies sequence order in barriers, the intervals (6) also naturally change.

For non-overlapped areas of barriers phonon frequencies the interface phonons frequencies are within the intervals

$$\omega_{TO,l} < \omega_1 < \omega_{LO,l}$$

$$\omega_{TO,r} < \omega_2 < \omega_{LO,r}. \quad (7)$$

Two solutions, corresponding to frequencies

$$\omega_{TO,w} < \omega_{3,4} < \omega_{LO,w},$$

are not considered in the examined approximation. Clearly, the equation (5) does not accurately define the spectrum of interface phonons from intervals (6) and (7) at $qa \geq 1$. However, exactly in the area (4), as will be shown further, the observed phonon branches make the biggest contribution to electron-phonon interaction.

3. Electron-phonon interaction

As per data from study [12], let's get the expression for Hamiltonian of the electron-phonon interaction H_{int} in the examined structure. It can be expressed the same way as for symmetric structure [13]:

$$H_{\text{int},i} = \sum_{\mathbf{q}} \left(\frac{2\pi\omega_i e^2}{L^2} \right)^{1/2} \frac{\exp(i\mathbf{q}\rho)}{\sqrt{2q}} f_i(\mathbf{q}, z) F_i(q, \omega) \times \left(a_i(\mathbf{q}) + a_i^+(\mathbf{q}) \right), \quad (8)$$

where L^2 is the normalizing area of the quantum well, $a_i(\mathbf{q})$ and $a_i^+(\mathbf{q})$ are the operators of destruction and generation of phonons of the branch number i (four branches in full spectrum and two in the area $qa \ll 1$). Factor $f_i(\mathbf{q}, z)$ describes the distribution of excitation intensity in the direction perpendicular to quantum well plane. In the examined case inside the quantum well at $|z| \leq a/2$ it is given by

$$f_i(\mathbf{q}, z) = \gamma_i(\omega_i) e^{qz} + \gamma_i^{-1}(\omega_i) e^{-qz}, \quad (9)$$

where parameter γ_i is defined with the following expression:

$$\gamma_i(\omega_i) = e^{-qa} \frac{\varepsilon_w(\omega_i) - \varepsilon_l(\omega_i)}{\varepsilon_w(\omega_i) + \varepsilon_l(\omega_i)} = e^{qa} \frac{\varepsilon_w(\omega_i) + \varepsilon_r(\omega_i)}{\varepsilon_w(\omega_i) - \varepsilon_r(\omega_i)}. \quad (10)$$

Expression (9) for $f_i(\mathbf{q}, z)$ differs from the similar expressions for structures with symmetrical barriers since in this case it is not possible to single out the symmetrical and asymmetrical modes.

The biggest difference from symmetrical structures is for coefficients $F_i(q, \omega_i)$:

$$F_i^{-1}(q,\omega_i) = \Big[\beta_l^{-1}(\omega_i)\{\gamma_i^2(\omega_i)e^{-qa} + 2 + \gamma_i^{-2}(\omega_i)e^{qa}\}$$
$$+\beta_r^{-1}(\omega_i)\{\gamma_i^{-2}(\omega_i)e^{-qa} + 2 + \gamma_i^2(\omega_i)e^{qa}\}$$
$$+\beta_w^{-1}(\omega_i)\left\{(e^{qa}-e^{-qa})\left(\gamma_i^2(\omega_i)+\frac{1}{\gamma_i^2(\omega_i)}\right)+2qa\right\}\Big]^{-1/2}. \quad (11)$$

Expression (11) describes the charged particles interaction with all branches of interface phonons. Here, the function $\beta_i(\omega_i)$ is given by [12]

$$\beta_i(\omega) = \left[\frac{1}{\varepsilon_{i,\infty}} - \frac{1}{\varepsilon_{i,0}}\right]\frac{\omega_{LO,i}^2}{\omega^2}\left[\frac{\omega^2-\omega_{TO,i}^2}{\omega_{LO,i}^2-\omega_{TO,i}^2}\right]^2. \quad (12)$$

From expression (11) it can be seen, that at $qa \ll 1$ the main contribution is made by the interaction, containing parameters $\beta_l(\omega)$ and $\beta_r(\omega)$, that are defined with dielectric properties of the barriers materials. Contributions, conditioned by properties of quantum well material and containing function $\beta_w(\omega)$, appear only in higher orders as per parameter (4). Expressions (9) and (11) are significantly simplified if condition (4) is met. In the highest order as per parameter (4) the constant of electron-phonon interaction α_k (equivalent of Frelich constant for volume materials) can be presented as:

$$\alpha_i = e^2\left(\frac{m}{2\omega_i}\right)^{1/2} R_{\text{as}}(\omega_i), \quad (13)$$

where $i = 1, 2$, m is the carriers mass in quantum well, while the last factor R_{as} is given by

$$R_{\text{as}}(\omega_i) = \left|F_i(q\omega_i) f_i(\mathbf{q}, z)\right|^2 \cong \frac{2\beta_r(\omega_i)\beta_l(\omega_i)}{\beta_r(\omega_i)+\beta_l(\omega_i)}. \quad (14)$$

Expression (14) means that in sufficiently narrow quantum wells the energy of electron-phonon interaction can be presented as a value constant over the well width. This value corresponds to polarization created by barriers. In sufficiently narrow quantum wells this polarization slightly changes with the well width. At the same time, the difference in spatial position of interaction maximums for ω_1 and ω_2 becomes insignificant. Dielectric properties of the quantum well material under this approximation also become insignificant. Expression for parameter $R_{\text{as}}(\omega_i)$ should be compared with the similar expression $R_{\text{sim}}(\omega_i)$, appearing at determination of the constant of electron-phonon interaction in symmetric quantum wells. It was shown earlier [3], that in symmetrical structures, if the conditions (4) are met, this value is equal to

$$R_{\text{sim}} = \frac{1}{\varepsilon_{\text{opt}}} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}, \quad (15)$$

where values of ε_∞ and ε_0 are related to barriers material. At the same time, the frequency of the interface mode is close to frequency ω_{LO} of longitudinal optical phonons of the barrier materials, and that results in expression (15). Expressions $R_{\text{sim},r}(\omega_i)$ and $R_{\text{sim},l}(\omega_i)$ will correspond to the quantum well, where the material of the right (r) or left (l) barriers of asymmetric structure will be used for both barriers.

In case of asymmetric structures with various barriers the phonon frequency will be different from both $\omega_{LO,l}$ and $\omega_{LO,r}$. While this difference is rather low, it should be considered for correct determination of electron-phonon interaction parameters. Figures 1 and 2 show the model calculations for parameters of $R_{\text{as}}(\omega_i)$ at various ratios of

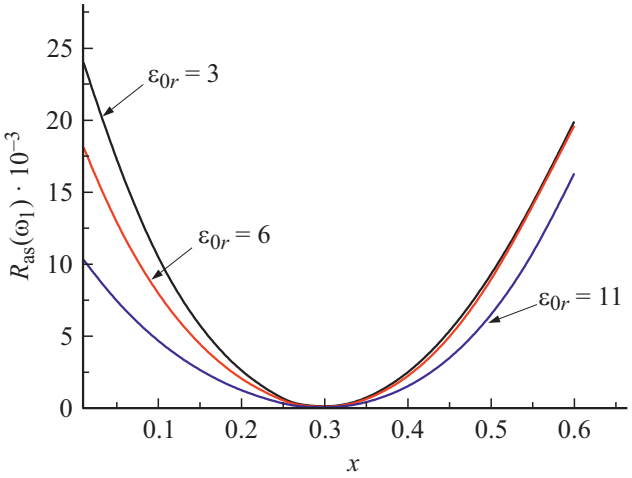

Figure 1. Dimensionless parameter of the electron-phonon interaction $R_{\text{as}}(\omega_1)$ at variation of the barriers dielectric properties. Model dependencies are used for barriers phonon frequencies $\omega_{LOl} = 1.8\omega_{TOl}$, $\omega_{TOr}(x) = (1.3 - x)\omega_{TOl}$, $\omega_{LOr}(x) = (1.5 + x)\omega_{TOl}$; $\omega_{TOl} < \omega_1 < \omega_{TOr}$; $\varepsilon_{0l} = 4$.

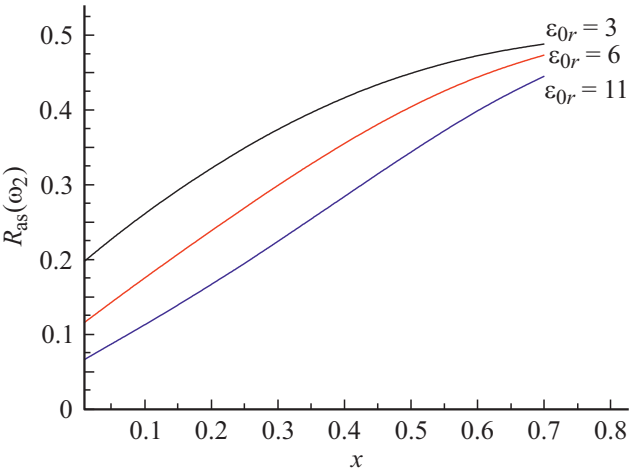

Figure 2. Dimensionless parameter of the electron-phonon interaction $R_{\text{as}}(\omega_2)$ at variation of the barriers dielectric properties. Model dependencies are used for barriers phonon frequencies $\omega_{LOl} = 1.8\omega_{TOl}$, $\omega_{TOr}(x) = (1.3 - x)\omega_{TOl}$, $\omega_{LOr}(x) = (1.5 + x)\omega_{TOl}$; $\omega_{LOl} < \omega_2 < \omega_{LOr}$; $\varepsilon_{0l} = 4$.

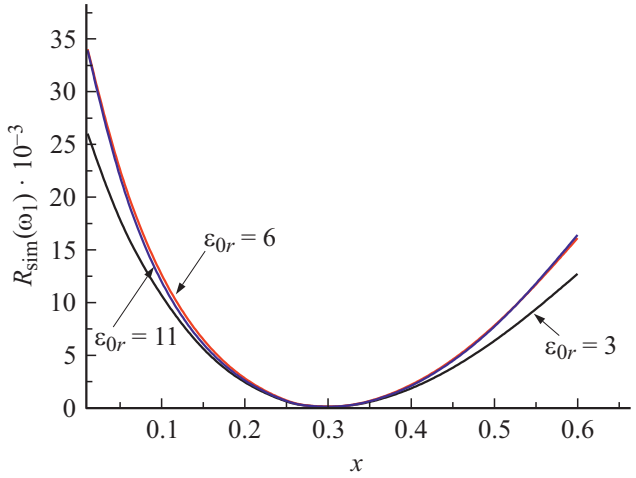

Figure 3. Dimensionless parameter of the electron-phonon interaction $R_{sim}(\omega_1)$ for the same barriers of r type with the same model dependencies of frequencies for the right barrier, as in Figs. 1 and 2.

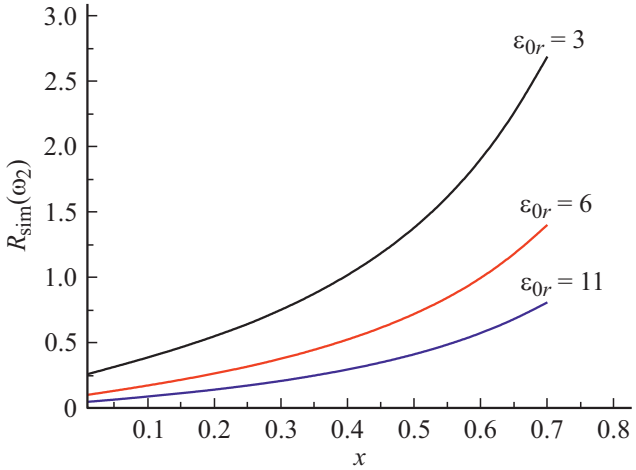

Figure 4. Dimensionless parameter of the electron-phonon interaction $R_{sim}(\omega_2)$ for the same barriers of r type with the same model dependencies of frequencies for the right barrier, as in Figs. 1 and 2.

the phonon frequencies of the barrier materials. The case is examined when the areas of the barriers phonon frequencies overlap. Linear dependence of phonon frequencies on some external parameter can be implemented using solid solutions of various composition as the barriers. As seen from Figs. 1 and 2, the interaction with one of the interface phonon modes exceeds another by one–two orders of magnitude. This is related to the fact that frequency ω_1 is between two TO-modes of barrier frequencies and it is close to similar parameters of transversal oscillations in terms of electron-phonon interaction parameter. Figures 3 and 4 show the values of dimensionless parameter of electron-phonon interaction $R_{sim}(\omega_i)$ for symmetric quantum wells with the same values of phonon frequencies, that were used in Figs. 1 and 2 for the left barrier. It can be seen that the values of electron-phonon interaction parameter are higher than for asymmetric structures. The parameter itself can change its value by several times. At the same time, at low values of static dielectric permittivity of the barriers the biggest changes are made in symmetric structures. At large values of ε_0, on the contrary, the major changes are typical for asymmetric structures. This allows to select an optimum method for electron-phonon interaction control for structures with various barriers.

Different situation is observed in case of non-overlapped areas of the barriers phonon frequencies. Figure 5 shows the model calculations of parameter $R_{as}(\omega_i)$ for this case. It should be noted that contributions of both phonon modes to electron-phonon interaction become similar in terms of value. Values of interaction parameters in this case can also change by several times. However, at close values of the phonon frequencies the interaction for carriers in quantum well with symmetric barriers is still higher.

Different situation is observed at significantly different phonon frequencies of the barriers. In this case we can perform the analytical comparison of parameters $R_{as}(\omega_i)$ and $R_{sim}(\omega_i)$. Let's for definiteness assume that $\omega_{LO,l} \gg \omega_{LO,r}$. Then, for interface phonons with frequency ω_1 close to $\omega_{LO,l}$, $\beta_l \ll \beta_r$,

$$R_{as}(\omega_i) \approx 2\beta_i(\omega_1). \tag{16}$$

In case of meeting the condition

$$\varepsilon_{r,\infty} < \frac{1}{2}\left[\left(\varepsilon_{l,0}^2 + \varepsilon_{l,\infty}^2 + 6\varepsilon_{l,0}\varepsilon_{l,\infty}\right)^{1/2} - (\varepsilon_{l,0} + \varepsilon_{l,\infty})\right], \tag{17}$$

we get

$$R_{as}(\omega_i) > R_{sim,l}(\omega_i). \tag{18}$$

This means that in asymmetric structure the electron-phonon interaction is higher than in symmetric, where both

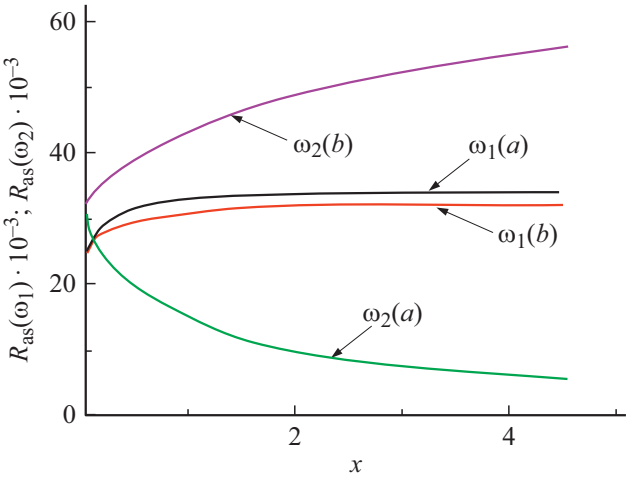

Figure 5. Values of $R_{as}(\omega_1)$ and $R_{as}(\omega_2)$ at non-overlapped areas of phonon frequencies for asymmetric barriers $\omega_{TO,l} < \omega_1 < \omega_{LO,l}$ and $\omega_{TO,r} < \omega_2 < \omega_{LO,r}$; a — $\omega_{LO,l} = \sqrt{2}\omega_{TO,l}$, $\omega_{TO,r} = (1.4 + x)\omega_{TO,l}$, $\omega_{LO,r} = (1.5 + x)\omega_{TO,l}$; b — $\omega_{LO,l} = \sqrt{2}\omega_{TO,l}$, $\omega_{TO,r} = (1.4 + x)\omega_{TO,l}$, $\omega_{LO,r} = (1.5 + 1.2x)\omega_{TO,l}$.

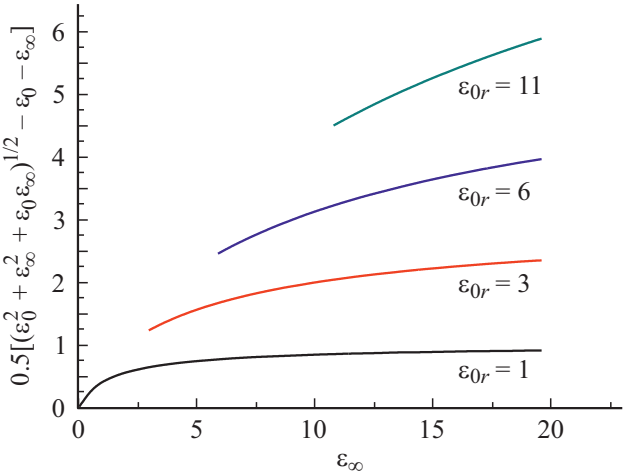

Figure 6. Boundary of the enhancement area for maximum asymmetrical barriers at various values of ε_{0r}.

barriers are made of material of the left barrier for the quantum well, examined in this study. At the same time, in asymmetric structure there is the second contribution in the area of low frequencies $\omega_{TO,r} < \omega_2 < \omega_{LO,r}$. For that area, usually, $\beta_l(\omega_2) \gg \beta_r(\omega_2)$, $R_{\text{as}}(\omega_2) \approx 2\beta_r(\omega_2)$ and condition

$$R_{\text{as}}(\omega_i) > R_{\text{sim},r}(\omega_i) \tag{19}$$

is implemented if the following relation is fulfilled

$$\varepsilon_{l,0} < \frac{1}{2}\left[\left(\varepsilon_{r,0}^2+\varepsilon_{r,\infty}^2+6\varepsilon_{r,0}\varepsilon_{r,\infty}\right)^{1/2}-(\varepsilon_{r,0}+\varepsilon_{r,\infty})\right], \tag{20}$$

Basically, the conditions (17) and (20) do not contradict each other and can be implemented simultaneously. However, if both barriers are made of materials with high level of ionicity, it is not possible to simultaneously implement the significant difference of phonon frequencies and fulfillment of conditions (17) and (20). However, there is a situation, when asymmetric barriers use creates higher polarization in the quantum well area, than if there are symmetric barriers. This is possible, if one of the barriers is made of low-polar or non-polar material with low value of dielectric permittivity. We will call such structure the quantum well with maximum asymmetric barriers. In this case the satisfaction of one of the inequalities — (17) or (20), depending on which barrier is made of non-polar material, is enough for the enhancement interaction. Also, one of the frequencies of the interface phonons becomes zero and the condition of the significant difference of frequencies is automatically met. Figure 6 shows the boundary of the enhancement area for various values of polar barrier parameters. At various values of ε_0 this boundary changes from $(\sqrt{2}-1)\varepsilon_\infty$ to ε_∞. To achieve the enhancement interaction the dielectric permittivity of the non-polar barrier should be less that this value.

In all other cases the biggest value of the electron-phonon interaction of polar type is implemented in structures with symmetric barriers with the highest level of ionicity. It should be noted that value of the electron-phonon interaction in the structures with various barriers changes by several times. This allows to potentially implement and study the transition from low to strong interaction. For that the material of at least one of the barriers should have high level of ionicity, that is required for generation of polarons of higher radius.

4. Conclusion

Thus, the use of barriers, asymmetric in terms of their dielectric parameters, for quantum well results in significant change of interaction of charged particles with polar optical phonons. Dimensionless parameter of interactions in such structures can change by several times. This should be considered at studying the processes of hot carriers relaxation, studying the optical and transport properties of similar structures. The possibility of interaction enhancement using non-polar materials as one of the barriers is of special interest. This opens additional possibilities for implementation of conditions for higher-radius polarons existence.

Conflict of interest

The authors declare that they have no conflict of interest.

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