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

© A.Yu. Maslov, O.V. Proshina

Ioffe Institute,
194021 St. Petersburg, Russia
E-mail: maslov.ton@mail.ioffe.ru

Received May 28, 2024
Revised September 19, 2024
Accepted September 19, 2024

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.

DOI: 10.61011/SC.2024.07.59544.6747

1. Introduction

Heterostructures fabricated of layers of materials of various ionicity have come into common use in recent years. In such structures, a number of new effects arise due to the transfer of phonon polarization between layers. In our previous papers [1,2] it was shown that in a quantum well with barriers of ionic materials, a strong interaction of charged particles with polar optical phonons may occur. At that, the presence of intrinsic polar phonons localized in the quantum well does not play any significant role.

On the other hand, heterostructures of the opposite type are also of considerable interest to researchers — when the quantum well is made of ionic material, and the barriers are made of nonionic or weakly ionic material. Such structures occur, primarily, when studying the extremely narrow layers of dichalcogenides of transition metals [3]. In particular, significant discrepancy between the carriers effective mass obtained from theoretical analysis and that measured experimentally was noted [4,5]. In our opinion, this discrepancy may be due to the fact that „polar“ mass of electron was measured, which may significantly differ from the „bare“ mass [6]. Earlier, other mechanisms of effective mass change related to the symmetry of the structure electronic states [7], the interline scattering of carriers on phonons [8] and specifics of the carriers interlayer interaction [9] were discussed. The mechanism outlined in this paper for changing the carriers effective mass is typical for any quantum wells based on ionic materials and, under certain conditions, can lead to significantly greater changes in its magnitude.

In this paper, the possibilities of changing the polaron mass of carriers in quantum well nanostructures based on ionic material are investigated. It is shown that for different nonionic barriers, with the same composition of ionic quantum well, significant changes in the magnitude of the polaron mass of the carriers can be obtained. This provides additional capabilities in studying the intrinsic physical properties of thin layers of ionic materials. The applicability of the proposed model to describe extremely thin layers of transition metal dichalcogenides is discussed.

2. Interaction attenuation factor

Let's consider a three-layer structure consisting of a narrow quantum well based on an ionic material surrounded by two barriers for charge carriers. The width of the quantum well a is suggested to be microscopic and exceeding the lattice constant. Also, the non-ionic barriers are assumed as microscopic. Such structure, of course, is not Van der Waals structure [10]. However, in our opinion its properties shall be taken into account also when studying the Van der Waals structures.

In such a structure, carriers can interact with a very large (formally infinite) number of polar phonon modes. Therefore, the approach proposed by Pekar for bulk materials turns out to be a convenient method for describing the electron-phonon interaction [11]. Further studies [12] demonstrated that Pekar's method provides a correct dependence of polaron effects on the material parameters in cases when interaction of charged particles with the phononic branches has one and the same order of magnitude. It is this case, that is implemented in this structure. The use of more complex methods provides only a slight refinement of the numerical coefficients in the formulas obtained. Following

the data of [11], we will describe the phonon field by the macroscopic potential of a polarized medium. Then, Schrödinger equation for a charged particle in a quantum well, taking into account the polarization of the medium, may be written as

$$\left[\widehat{H_0} + U(\mathbf{r}) + \frac{\varepsilon_{\text{opt}}^{(w)}}{8\pi} \int\limits_{|z|<a/2} d^3r \left|\nabla U(\mathbf{r})\right|^2 + \frac{\varepsilon_{\text{opt}}^{(b)}}{8\pi} \int\limits_{|z|>a/2} d^3r \left|\nabla U(\mathbf{r})\right|^2\right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \qquad (1)$$

where $\widehat{H_0}$ — Hamiltonian of an electron in the quantum well neglecting the polarization, $\varepsilon_{\text{opt}}^{(i)} = \left[\frac{1}{\varepsilon_\infty^{(i)}} - \frac{1}{\varepsilon_0^{(i)}}\right]^{-1}$ — optical dielectric permittivity. Symbol i turns into value „w“ in the quantum well and „b“ in barriers, a — width of the quantum well, axis z oriented perpendicular to the well plane. Equation (1) obviously may be summarized for the case of two different barriers. In this paper, we will adhere to the case when the effect of barrier polarization on the overall polarization of the structure can be ignored, and assume $\varepsilon_{\text{opt}}^{(b)} = 0$. Let's average out the expression (1) on the unknown wave function of electron $\Psi(\mathbf{r})$ and find the extremum of the phonon field potential. This potential satisfies the equation that is standard for the large-radius polaron problem:

$$\Delta U(\mathbf{r}) = \frac{4\pi e}{\varepsilon_{\text{opt}}^{(w)}} \left|\Psi(\mathbf{r})\right|^2; \quad |z| < \frac{a}{2}. \qquad (2)$$

This approach is applicable only if the radius of the polaron exceeds the lattice constant. We will assume that a more stringent condition is fulfilled when the radius of the polaron turns out to be greater than the width of the quantum well a, i. e.

$$r_p > a. \qquad (3)$$

Then, in equation (1) the motion of the charged particles along z axis is defined by the intrinsic potential of the quantum well, and the full wave function may be presented as a production of the two functions, one of which depends only on z, and the other one depends on the 2D vector $\boldsymbol{\rho}$ in the plane of the well:

$$|\Psi(r)| = |\psi(z)|\chi(\boldsymbol{\rho}). \qquad (4)$$

By averaging the equation (1) in the wave function (4) taking into account (3), we'll obtain the polaron energy shift ΔE_{pol} as follows:

$$\Delta E_{\text{pol}} = -\frac{e^2 f}{2\varepsilon_{\text{opt}}^{(w)}} \int d^2\boldsymbol{\rho}' \frac{|\chi(\boldsymbol{\rho}')|^2}{|\boldsymbol{\rho} - \boldsymbol{\rho}'|}, \qquad (5)$$

where the dimensionless multiplier f is implied as a portion of the transverse motion electron density limited by the width of the quantum well:

$$f = \int\limits_{-a/2}^{a/2} dz \left|\psi(z)\right|^2. \qquad (6)$$

From the 2D polaron theory [13] it is known that equation (5) may be solved through a universal dimensionless function that was numerically calculated many times. At that, additional multiplier f which appears in equation (5) results in occurrence of the efficient interaction parameter $\alpha_{\text{eff}} = \alpha_0 f$, where α_0 — „bare“ dimensionless interaction parameter. This value plays a decisive role in our review. For a quantum well with infinite barriers, the transverse motion wave function is localized inside the well, and the parameter $f = 1$. At that, the equation (5) delineates the standard energy of polaron shift in the two-dimensional system [12]. But for any quantum well of finite depth this parameter turns out to be less than a unit. This means that the effective parameter of the electron-phonon interaction decreases proportionally to the multiplier f and, depending on the height of potential barriers, can take any values from one to almost zero. It should be noted that in the review the enhancement of the electron-phonon interaction [1,2], taking into account the finite depth of the well, leads to minor corrections, which, as a rule, may be ignored. Major contribution to the enhanced interaction is provided by the interface phonons and their properties. In this case, the interaction of charged particles with interface phonons turns out to be parametrically large.

In the reviewed case the situation turns out to be quite opposite. Interaction with interface phonons is not distinguished by anything [14] and practically does not affect weakening of the total electron-phonon interaction. But the „leakage“ of the part of the electron density outside the quantum well turns out to be important. It is this factor, that leads to potential weakening of the interaction. We don't know any other mechanisms that could lead to a weakening of the interaction of charged particles with polar optical phonons in a quantum well made of ionic material. As the simplest example, we can consider a rectangular potential well with barriers of height u_0. This problem was studied in details in many books on quantum mechanics, e.g., in book [15]. By using the well-known equations for the wave function $\psi(z)$, we may obtain for the multiplier f the following expression:

$$f = \frac{q}{q+1}\left[1 + \frac{q}{q^2 + k^2}\right], \qquad (7)$$

where

$$k = \frac{a\sqrt{2mE_n}}{\hbar}; \quad q = \frac{a\sqrt{2m(u_0 - E_n)}}{\hbar}, \qquad (8)$$

E_n — value of n-th level of the electron energy in the well.

For the states $\psi(z)$ symmetrical in terms of the wave function the energy is found by solving the transcendental equation

$$\operatorname{tg} k = \frac{q}{k}, \tag{9}$$

and for the antisymmetric states it is found from the equation

$$\operatorname{tg} k = -\frac{k}{q}. \tag{10}$$

It is interesting to mention, that dependence of the weakening multiplier f on parameters q and k is defined by equation (7) and remains the same for both types of states from equations (9) and (10).

The multiplier f weakening the electron-photon interaction from equation (7) depends on the carriers' mass m^*, quantum well width a and its depth u_0. The position of the electron energy level E_n turns out to be an auxiliary parameter in this case, which is not included explicitly in equation (7).

Figure 1 shows the dependencies of multiplier f on the well depth u_0 for several characteristic values of the well width a.

As expected, a significant weakening of the electron-phonon interaction occurs in sufficiently narrow and not too deep potential wells when the height of the barrier is less than the width of the band gap. For certainty, we used in our calculations the value of „bare" effective mass (in units of the mass of the free electron m_0) $m^* = 0.4m_0$. „The bare" mass cannot be determined experimentally and is in a sense a fitting parameter of the problem. This value was selected because such mass corresponds to MoS_2compound [16].

An effective mass close to this value is typical for a number of other transition metal dichalcogenide compounds. Figure 2 illustrates the dependencies of the multiplier f for the first excited state of the electron (if it can exist due to the well parameters) on the well depth u_0.

At that, the obtained values f with the same well parameters turn out to be sufficiently less than for the ground state of the electron. This means that within the framework of our proposed model, the magnitude of the electron-phonon interaction for excited states should be less than for the ground state. In all the above calculations, the condition of applicability of the proposed model (3) turned out to be fulfilled.

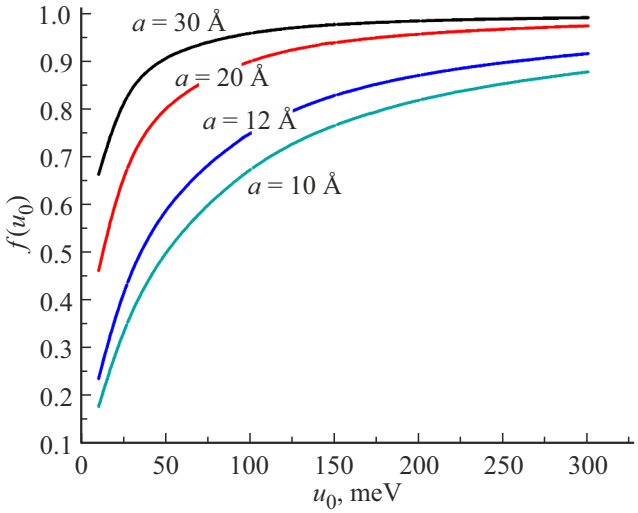

Figure 1. The dependencies of the weakening multiplier f on the well depth u_0 for the ground state of the electron in the quantum wells of various width a.

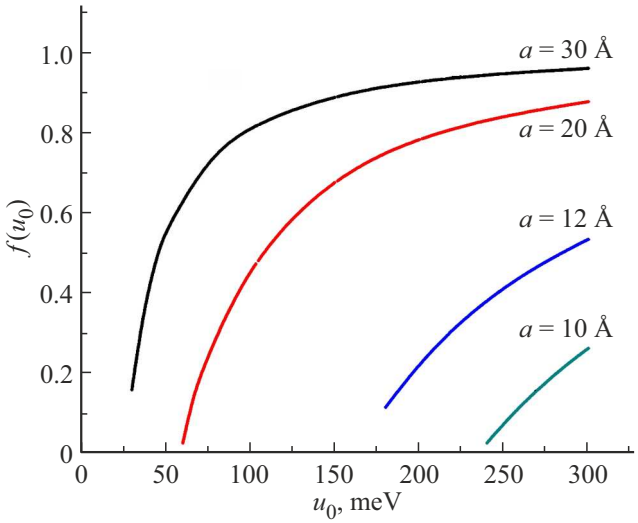

Figure 2. The dependencies of the weakening multiplier f on the well depth u_0 for the first excited state of the electron in the quantum wells of various width a.

3. Carriers polaron mass

The predictions of the proposed model can be experimentally verified from measurements of the „polaron" mass of charge carriers in the considered structures. If there's a significantly strong electron-phonon interaction, the effective mass of the carriers greatly depends on the dimensionless interaction parameter α_0. Analytical expressions for such a dependence in two-dimensional systems are given in [17]. We believe that in the considered structures the expressions for the polaron mass of the charge carriers should include an effective interaction parameter α_{eff} equal to

$$\alpha_{\text{eff}} = f\alpha_0, \tag{11}$$

which is less than the intrinsic parameter of the quantum well material α_0 because of the weakening multiplier f from the equation (7). Then, the equations for the carriers polaron mass outlined in paper [16] will look as follows:

$$m_{\text{pol}} = m^*\left(1 + \frac{\pi}{8}\alpha_{\text{eff}}\right) \quad \text{by} \quad \alpha_{\text{eff}} < 1, \tag{12}$$

$$m_{\text{pol}} = 0.733m^*\alpha_{\text{eff}}^4 \quad \text{by} \quad \alpha_{\text{eff}} > 1. \tag{13}$$

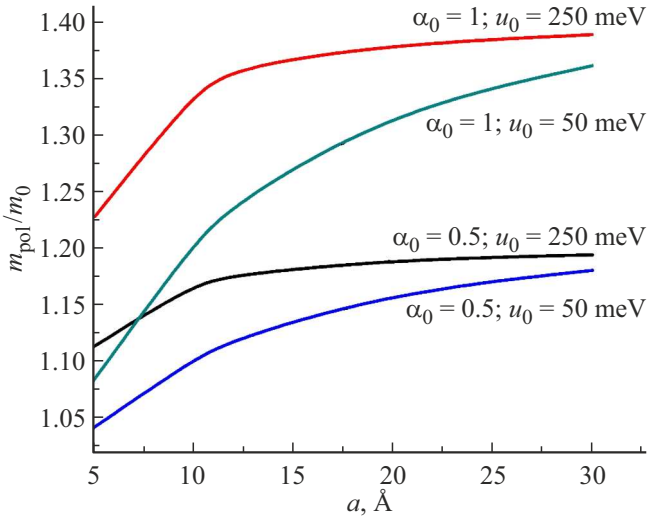

Figure 3. The dependencies of the carriers polaron mass m_{pol}/m_0 on the quantum well width a for the values of interaction intrinsic parameter $\alpha_0 \leq 1$.

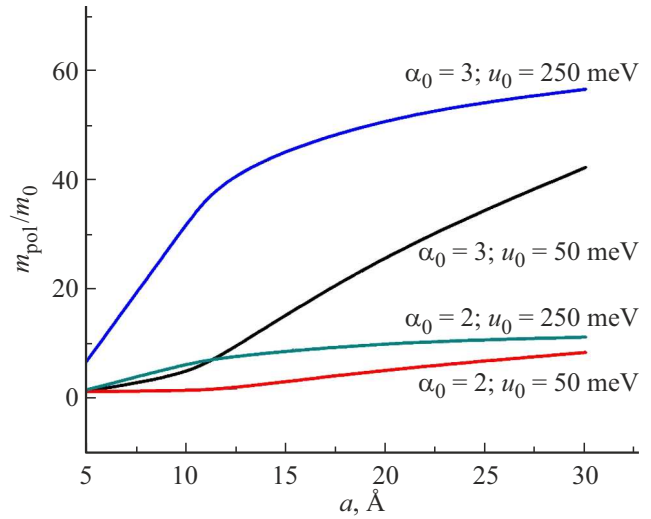

Figure 4. The dependencies of the carriers polaron mass m_{pol}/m_0 on the quantum well width a for the values of interaction intrinsic parameter $\alpha_0 > 1$.

Figure 3 and 4 illustrate the dependencies of the polar mass of carriersm_{pol} on the quantum well width a for several values of the interaction intrinsic parameter α_0. „Cross-linking“ of equations (12) and (13) occurs at $\alpha_{eff} = 1.18$, which was taken into account. Certainly, the use of formula (12) at $\alpha_{eff} \gtrsim 1$ is not fully correct. But, since corrections for the effective mass in the domain of weak electron-phonon interaction are not high, it is unlikely it may cause any significant errors in the given results.

From Figure 3 we may see that even at relatively low interaction ($\alpha_0 \leq 1$) there's a visible dependence of the polaron mass m_{pol} on the quantum well width a. This dependence turns out to be significant for compounds with their intrinsic interaction parameter α_0 exceeding one (Figure 4). We believe that experimental confirmation of the dependence of the carriers effective mass on the quantum well width is the most realistic way to verify the proposed model.

4. Results and discussion

In this paper, it is shown that in structures consisting of an ion material quantum well surrounded by not very high barriers of nonionic material, the effect of suppression of the electron-phonon interaction inside the well occurs. The magnitude of this suppression effect is calculated depending on the height of the barriers and the width of the quantum well. It is shown that this effect leads to a dependence of the effective mass of the carriers on the structure parameters. A particularly strong dependence is expected for compounds for which the intrinsic parameter of the electron-phonon interaction exceeds one.

It follows from our consideration that the effective mass of carriers in the excited state should be less than in the ground state due to decline in the magnitude of the weakening multiplier f from equation (7). This effect is determined by the general properties of wave functions in a finite depth well and does not depend on the specific shape of the quantum well. Because this effect was found experimentally it may serve as an additional way of verifying the proposed model.

5. Conclusion

Our problem was solved within the framework of a continuum model, where the width of the quantum well was considered as a continuous parameter. However, all the approximations made in this paper make it possible to apply the results also to an extremely narrow quantum wells consisting of one or more monolayers of an ionic compound. At that, the dielectric barriers should be considered macroscopic. In particular, it should be expected that, when using in the considered structures the layers of transition metal dichalcogenides as a quantum well, the dependence of the effective mass of carriers on the number of layers may be observed. To quantify this effect, a more accurate description of the shape and parameters of the quantum well, as well as possible changes in the band structure of multilayer materials [18], may be required. However, in our opinion, the qualitative patterns obtained in this study should be preserved. It should also be emphasized that the results obtained cannot be used to describe the properties of Van der Waals structures. That being said, the predictions about the dependence of the carriers' effective mass on some parameters of the barriers surrounding the well can also be useful for understanding the properties of structures consisting of monoatomic layers of various materials.

Conflict of interest

The authors declare that they have no conflict of interest.

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Translated by T.Zorina