Chapter 1

Interface Phonons and Polaron States in Quantum Nanostructures

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Additional information is available at the end of the chapter

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Abstract

The interface optical phonons arise near the hetero-interface of a quantum nanostructure. Moreover, its spectrum and dispersion laws may differ from ones for excitations arising in the bulk materials. The study of such excitations can give fundamentally new information about the optical and transport properties of nanostructures. The interaction of charged particles with polar optical phonons can lead to the large radius polaron creation in the materials with high ionicity. This chapter deals with the results of our theoretical investigations of the polaron states in quantum wells, quantum wires, and quantum dots. The charged particle and exciton interaction with both bulk and interface optical phonons are taken into account. The original method has been developed taking into consideration an interface phonon influence. The enhancement conditions are found for both strong and weak interactions. It is established that the barrier material dielectric properties give a decisive contribution to the polaron binding energy value for strong electron-phonon interaction. The manifestation of strong polaron effects is a pronounced demonstration of the interface optical phonon influence on optical and transport properties of nanostructures.

Keywords: interface optical phonons, quantum well, quantum wire, quantum dot, electron-phonon interaction, polaron

1. Introduction

The electron-phonon interaction proves to be rather weak for most of the phonon branches. Such interaction can be taken into account in the framework of perturbation theory. The interaction of charged particles with polar optical phonons turns out to be fundamentally different [1]. The effective constant of the electron-phonon interaction may exceed unity in

materials with high ionicity. Moreover, the formation of a new type of elementary excitations, which is a bound state of charged particles and polar optical phonons, is possible even in bulk materials. This is the so-called large-radius polaron. The conditions for the appearance of such polaron are most favorable in quantum-dimensional structures. First, the additional branches of polar optical phonons, which are the interface phonons, appear in such structures. Second, the effective interaction of charged particles with polar optical phonons increases with the decreasing structure dimensionality. This significantly expands the range of materials for the nanostructure design where the large-radius polaron formation is possible. The large-radius polaron appearance significantly changes the optical and transport properties of nanostructures. Even the manifestation of polaron superconductivity may take place [2]. Available theoretical studies of large radius polaron in quantum nanostructures consider the charged particle interaction with only one polar phonon mode [2–10]. This approach seems to be inconsistent for us. The phonon spectrum modification turns out to be very significant in quantum nanostructures. Therefore, it is necessary to take into account the interaction with all phonon branches in the large-radius polaron investigations.

In this chapter, conditions of strong electron-phonon interaction observation are investigated theoretically in the quantum well, quantum wire, and quantum dot. Particular attention is paid to the theory of charged particle interaction with interface optical phonons playing a decisive role in quantum wells and quantum wires. The contribution of interface phonons to the interaction energy value turns out to be comparable with that of bulk phonons in the quantum dot case. The conditions necessary for the strong electron-phonon interaction are obtained for all types of nanostructures. Analytic expressions for the polaron binding energy are found for nanostructures considered. In some cases, the results for the weak electron-phonon interaction are discussed. This helps to understand better the interaction in a region of intermediate values of the coupling constant where obtaining the analytical result is impossible.

The total Hamiltonian of the system is given by:

$$\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{e-ph,} \tag{1}$$

where the electron Hamiltonian $\hat{H}_e$ describes charged particle interaction with nanostructure potential; $\hat{H}_{ph}$ contains the energies of all optical phonon branches; and $\hat{H}_{e-ph}$ is the electron-phonon interaction Hamiltonian. The expressions for these operators will be given below. The wave functions and energies corresponding to the Hamiltonian from Eq. (1) can be found both for the strong and for the weak electron-phonon interaction. Strong interaction is implemented under the condition:

$$E_{pol} \gg \hbar\omega_0. \tag{2}$$

Here $\hbar\omega_0$ is the optical phonon energy and E_{pol} is the polaron binding energy. Weak interaction corresponds to the inverse inequality:

$$\hbar\omega_0 \gg E_{pol}. \tag{3}$$

In this case, the contribution of the electron-phonon interaction can be taken into account by perturbation theory.

The adiabatic approximation turned out to be an effective method for solving the problem in the case of a strong electron-phonon interaction. Within the framework of this approach, the motion of the charged particles (electrons and holes) is considered to be fast, and vibrations of the atoms of the crystal lattice are supposed to be slow. The Hamiltonian from Eq. (1) can be averaged over the wave function of fast motion Ψ_m. The averaged Hamiltonian $\hat{H}_{av}$ can be written in the form:

$$\hat{H}_{av} = E_m\{\Psi_m\} + \hat{H}_{ph} + \hat{H}_{e-ph,av}. \tag{4}$$

Eq. (4) contains the energy of charged particles $E_m\{\Psi_m\}$, which is the functional of the wave function in a general case. Here $\hat{H}_{e-ph,av}$ is the Hamiltonian of electron-phonon interaction averaged over the wave function Ψ_m. In what follows, we will use the standard expression for $\hat{H}_{ph}$:

$$\hat{H}_{ph} = \sum_{r,n} \hbar\,\omega_{r,n}\, a^{+}_{r,n}\, a_{r,n}, \tag{5}$$

where the index r denotes different phonon branches; n is the quantum number that takes various values for the different nanostructures; $a^{+}_{r,n}$ and $a_{r,n}$ are the phonon creation and annihilation operators, respectively. Averaged Hamiltonian of electron-phonon interaction $\hat{H}_{e-ph,av}$ can be written as:

$$\hat{H}_{e-ph,av} = \sum_{r,n} \alpha(r,n)\left[a^{+}_{r,n} + a_{r,n}\right]. \tag{6}$$

Here the interaction parameters $\alpha(r,n)$ must be defined for all phonon branches in each nanostructure type. Eq. (4) is reduced to a diagonal form with respect to the phonon variables by using the unitary transformation $e^{-U}\hat{H}_{av}\,e^{U}$, where

$$U = \sum_{r,n} \alpha(r,n)\left[a_{rn} - a^{+}_{rn}\right]. \tag{7}$$

As a result, we get

$$e^{-U}\hat{H}_{av}\,e^{U} = E_{pol}\{\Psi_m\} + \hat{H}_{ph}. \tag{8}$$

As follows from Eq. (8), the spectrum of all phonon branches remains unchanged in the adiabatic approximation. The value $E_{pol}\{\Psi_m\}$ has the meaning of the binding energy of a large-radius polaron. This energy depends on the charge particle interaction parameters for all branches of the polar optical phonon spectrum. It is also a functional of the electron wave function Ψ_m that is used in the averaging procedure. The explicit form of this wave function Ψ_m is determined from the condition for the minimum of the polaron energy E_{pol}. This solution scheme is used below to find the polaron binding energy in various nanostructures.

2. Symmetric quantum well

In general, for the case of a quantum well, the interaction of charged particles with the phonons of the well, barriers, and interface phonons must be taken into account. Let us consider

the case of complete localization of charged particles within a quantum well. In this case, the interaction of such particles with barrier material phonons can be neglected. Nevertheless, the effect of barriers is very important. This is determined by the structure and properties of interface phonon spectrum. To describe the properties of interface phonons, we will use the continuum model proposed in [11]. The spectrum of the symmetric mode of interface phonons is determined from the solution of the following equation:

$$\varepsilon^{(w)}(\omega) th\left(\frac{qL}{2}\right) + \varepsilon^{(b)}(\omega) = 0, \tag{9}$$

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

$$\varepsilon(\omega) = \varepsilon_{\infty} \frac{\omega^2 - \omega_{LO}^2}{\omega^2 - \omega_{TO}^2}. \tag{10}$$

Here ω_{LO} and ω_{TO} are the frequencies of longitudinal and transverse optical phonons, respectively, and ε_{∞} is the high-frequency dielectric constant. The expression Eq. (10) means that we use the approximation of dispersionless modes for bulk optical phonons. It is in this approximation interface, and bulk phonon modes can be considered independently [12]. 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. Let us start with the electron polaron. The amplification of the electron-phonon interaction occurs in fairly narrow quantum wells having a width L that is less than the polaron radius a_0:

$$L < a_0. \tag{11}$$

The exact definition of the polaron radius a_0 will be given below.

When the inequality from Eq. (11) is satisfied, the electron wave function $\Psi_m^{(e)}(\mathbf{r})$ can be represented as a product:

$$\Psi_m^{(e)}(\mathbf{r}) = \phi_m(z)\, \chi_m(\mathbf{r}_{\parallel}), \tag{12}$$

where $\phi_m(z)$ is the transverse motion wave function that is determined by the quantum well potential; $\mathbf{r}_{\parallel}$ is the two-dimensional plane well coordinate; and $\chi_m(\mathbf{r}_{\parallel})$ is yet unknown two-dimensional wave function that is determined by electronic localization in a self-consistent well created by polar optical phonons.

The electron-phonon interaction parameters $\alpha(r, n)$ from Eq. (6) are given in [11, 13]. For further discussion, we will use an explicit form of these coefficients for the symmetric interface mode and an even part of the interaction with the localized phonons of the quantum well. Performing the aforementioned procedure allows us to get the polaron binding energy $E_{pol,well}$

from Eq. (8) as a functional of the wave function $\chi_n(\mathbf{r}_\parallel)$ for the quantum well case. It can be defined from the condition of minimum for this functional [13]:

$$-\frac{\hbar^2}{2m_e}\nabla^2\chi_m(\mathbf{r}_\parallel)-\frac{e^2}{\varepsilon_{opt}^{(b)}}\int d^2\mathbf{r}_\parallel\frac{|\chi_m(\mathbf{r}_\parallel)|^2}{|\mathbf{r}_\parallel-\mathbf{r}_\parallel'|}\chi_m(\mathbf{r}_\parallel)=\left(E_m-E_{pol,well}^{(e)}\right)\chi_m(\mathbf{r}_\parallel). \tag{13}$$

Here $E_{pol,well}^{(e)}$ is the electron polaron binding energy; $\varepsilon_{opt}^{(b)}$ from $\frac{1}{\varepsilon_{opt}^{(b)}}=\frac{1}{\varepsilon_\infty^{(b)}}-\frac{1}{\varepsilon_0^{(b)}}$ is the optical dielectric function of the barriers; and E_m is the size quantization level energy. Eq. (13) formally coincides with the equation for two-dimensional polaron [3–6, 14]. However, it should be noted that Eq. (13) involves the electron mass within the quantum well and the optical barrier dielectric constant. This combination of parameters appears because the major contribution to the polaron binding energy is given by interaction with interface optical phonons. In accordance with Eq. (13), the polaron binding energy in the quantum well is:

$$E_{pol,well}^{(e)}=-C_1\frac{m_e e^4}{\left(\varepsilon_{opt}^{(b)}\right)^2\hbar^2}, \tag{14}$$

where $C_1\cong 0.4$ is the numerical coefficient. Its value is determined by the integral of two-dimensional polaron dimensionless wave function $\chi_m(\mathbf{r}_\parallel)$ given in [14]. In this case, the radius of the electron polaron state $a_0^{(e)}$ is:

$$a_0^{(e)}=\frac{\hbar^2\varepsilon_{opt}^{(b)}}{m_e e^2}. \tag{15}$$

It is this quantity from Eq. (11) on which the adiabatic approximation used in our work is based. In the next order in the parameter from Eq. (11), some corrections to polaron binding energy Eq. (14) appear. These corrections can be expressed in terms of the dimensionless wave function of two-dimensional polaron $\chi_0(\mathbf{r}_\parallel)$ known from [14]. The calculations give the following:

$$\Delta E_{pol,well}=E_{pol,well}^{(e)}\frac{L}{a_0^{(e)}}\left(D_V+D_S\right)C_2, \tag{16}$$

where $C_2=0.07$ is the numerical factor that was calculated in [3]. The dimensionless coefficients D_V and D_S are determined by fairly complex combinations of the phonon frequencies in the quantum well and barrier materials and are found in [13]. It turns out that the corrections to the binding energy of a polaron are related to the interaction with both bulk and interface phonons. According to the expressions for D_V and D_S received in [13], these corrections may have different signs. The total value of the binding energy depends essentially on the dielectric properties of both the quantum well and the barrier materials. We note that the main contribution to polaron binding energy from Eq. (14) coincides with our result obtained earlier in [15] by means of an approximate method for calculating the phonon fields. However, the accurate inclusion of corrections to $E_{pol,well}^{(e)}$ in this approximate approach is impossible. Obtaining a quantity $\Delta E_{pol,well}$ from Eq. (16) requires taking into account the phonon spectrum of the system.

A similar consideration can be repeated for a hole polaron. The main contribution to the binding energy of a hole polaron is determined by an expression analogous to Eq. (14). It looks like this:

$$E_{pol,well}^{(h)} = -C_1 \frac{m_h e^4}{\hbar^2 \left(\varepsilon_{opt}^{(b)}\right)^2}. \tag{17}$$

Usually, for semiconductor materials, the hole mass m_h is much larger than the electron mass m_e, then the binding energy of the hole polaron from Eq. (17) is much larger than the energy of the electron polaron from Eq. (14). In this case, the localization region for a hole polaron $a_0^{(h)}$ turns out to be smaller than that for an electron polaron $a_0^{(e)}$:

$$a_0^{(h)} = \frac{m_e}{m_h} a_0^{(e)} << a_0^{(e)}. \tag{18}$$

The condition from Eq. (18) plays an important role in the study of a polaron exciton. The interaction of an exciton with optical phonons has a number of additional features. Polarization of the medium, created by an electron and a hole, partially compensates each other. The degree of this compensation essentially depends on the ratio of the radii of the electron and hole polarons, $a_0^{(e)}$ and $a_0^{(h)}$, respectively, and the exciton radius $a_0^{(ex)}$. In this case, the influence of the barrier dielectric properties on the exciton state must be taken into account in narrow quantum wells. Without allowance for the electron-phonon interaction, such influence was considered in [16]. In these articles, it was shown that the exciton binding energy in narrow symmetric quantum wells has the form:

$$E_{ex,well} = \frac{2\mu e^4}{\left(\varepsilon_0^{(b)}\right)^2 \hbar^2}. \tag{19}$$

Here μ is the reduced mass of the electron and hole in the quantum well. The radius of such quasi-two-dimensional exciton $a_0^{(ex)}$ also depends on the barrier dielectric constant $\varepsilon_0^{(b)}$. It is equal to:

$$a_0^{(ex)} = \frac{\hbar^2 \varepsilon_0^{(b)}}{\mu e^2}. \tag{20}$$

Eqs. (19) and (20) are valid for narrow quantum wells, the width of which satisfies the inequality

$$L < a_0^{(ex)}. \tag{21}$$

The possibility of strong coupling of an exciton with polar optical phonons depends on the relationship between $a_0^{(ex)}$ and $a_0^{(h)}$. It is seen from Eqs. (15) and (20) that the electron polaron radius is always greater than the exciton one, that is $a_0^{(e)} > a_0^{(ex)}$. If also $a_0^{(h)} > a_0^{(ex)}$, then the medium polarization created by the electron and hole largely compensates each other. In this case, for the exciton, the condition of strong coupling with phonons, as a rule, is not realized.

When the opposite relationship is satisfied, that is

$$a_0^{(h)} < a_0^{(ex)}, \tag{22}$$

the strong exciton-phonon interaction is possible. The main contribution to the polaron exciton binding energy is due to the localization of the hole in the polaron well. Its size is determined by the radius of the hole polaron $a_0^{(h)}$. The motion of an electron occurs in a larger region of space. The medium polarization created by the electron compensates partially the polarization created by the hole. If we take into account the largest contributions with respect to the parameters of Eqs. (11) and (22) only, then the polaron exciton binding energy is equal to:

$$E_{ex,well} = C_1 \frac{m_h e^4}{\hbar^2 \left(\varepsilon_{opt}^{(b)}\right)^2} - 2\frac{m_e e^4}{\hbar^2 \left(\varepsilon_{\infty}^{(b)}\right)^2}. \tag{23}$$

The second contribution in Eq. (23) is small, compared to the first one in the parameter $m_e/m_h \ll 1$. It can be seen from Eq. (23) that the possibility of strong coupling of an exciton with optical phonons depends on parameters of both the quantum well and barrier materials. The appearance of a polaron exciton requires a significant difference between the effective masses of an electron and a hole in a quantum well. In addition, the presence of barriers made of high ionicity materials is necessary. In this case, the polarization properties of the quantum well material do not play an essential role.

For most II–VI compounds, the exciton radius $a_0^{(ex)}$ from Eq. (20) is in the range 20–40 $\mathring{A}$. The electron polaron radius $a_0^{(e)}$ (Eq. (15)) falls within the range 50–100 $\mathring{A}$, and hole polaron one $a_0^{(h)}$ (Eq. (18)) is approximately 10–20 $\mathring{A}$. Therefore, the strong exciton-phonon interaction condition from Eq. (22) can be satisfied. This means that the quasi-two-dimensional polaron formation is possible in sufficiently narrow quantum wells of width $L < 20$ $\mathring{A}$.

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 [17]. In the III–V compounds, effective masses of quantum well carriers are small. The optical dielectric function of the barriers based on II–VI materials is also rather small. Thus, given above values of exciton and polaron radii increase by 2 – 3 times. Hence, a quasi-two-dimensional polaron in heterovalent quantum wells can be observed for the well widths $L \leq 50$ $\mathring{A}$. Quantum wells of more complex configuration (e.g., I–VII/III–V) can also become a promising object for the polaron study when strong electron-phonon interaction takes place.

3. Cylindrical quantum wire

In the quantum wires under consideration, the spectrum of interface phonons depends on the one-dimensional wave vector $\mathbf{q}$ directed along the wire axis. Using the same Eq. (10) for the dielectric functions of wire and barrier materials, we obtain the interface phonon spectrum equation in the context of the continuum approximation:

$$\frac{I'_m(q\,\rho_0)}{I_m(q\,\rho_0)}\,\varepsilon^{(b)}(\omega) = \frac{K'_m(q\,\rho_0)}{K_m(q\,\rho_0)}\,\varepsilon^{(w)}(\omega). \tag{24}$$

Here I_m is the m-th order modified Bessel function of the first kind; K_m is the m-th order modified Bessel function of the second kind; and ρ_0 is the quantum wire radius. The interface phonon spectrum is determined by solution of Eq. (24). The wave vector dependences of interface phonon frequencies are shown in **Figure 1**. These dependences are calculated for the quantum wire based on *CdSe*, surrounded by *ZnSe* barriers for $m = 0$ in Eq. (24). The compound parameters are taken from [18].

The adiabatic parameter of this problem is the ratio between the quantum wire radius ρ_0 and the polaron radius a_0:

$$\rho_0 \ll a_0. \tag{25}$$

Below, an exact analytic expression is obtained for determining the polaron radius. The inequality Eq. (25) means that the main contribution to the binding energy of a polaron is determined by the wave vector values which are small as:

$$q\,\rho_0 < 1. \tag{26}$$

According to Eq. (25), the electron wave function for n-th size quantization level can be written as:

$$\Psi^{(e)}(\mathbf{r}) = \phi(n^{(e)}; m^{(e)}; \boldsymbol{\rho})\chi(n^{(e)}; m^{(e)}; z)\, e^{im^{(e)}\phi}. \tag{27}$$

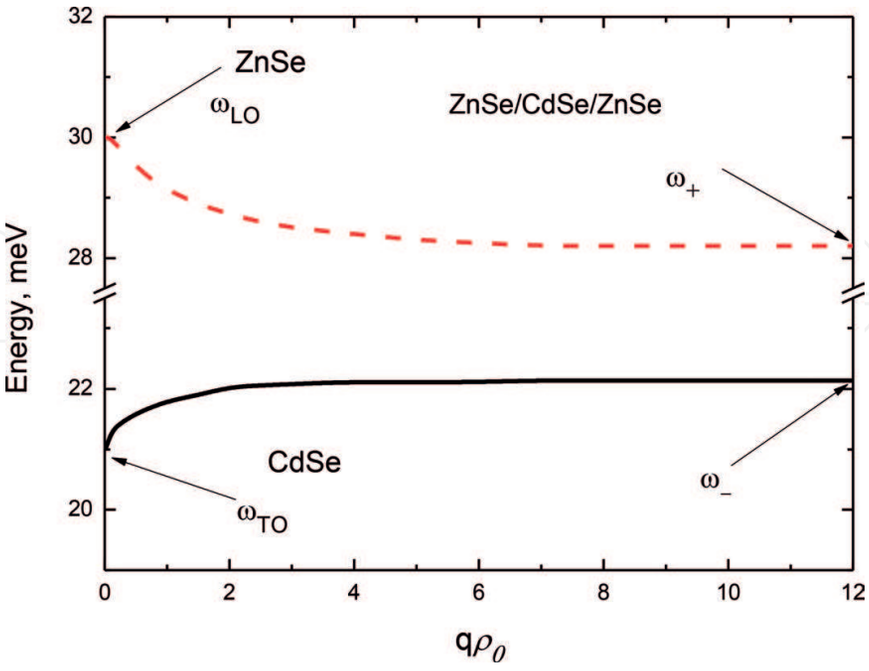

Figure 1 . Wave vector dependencies of interface optical phonon energies for *ZnSe/CdSe/ZnSe* quantum wire; $m = 0$.

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Here $n^{(e)}$ is size quantization level number and $\phi(n^{(e)}, m^{(e)}, \boldsymbol{\rho})$ is the wave function of two-dimensional electron motion. The electron-phonon interaction does not affect this motion, which occurs within a quantum wire. The wave function $\chi(n^{(e)}, m^{(e)}, z)$ describes the electron localization in phonon self-consistent potential well. Not disturbed electron states in the quantum wire are defined by the quantum numbers $n^{(e)}$ and $m^{(e)}$. In the case of total electron localization inside the cylindrical quantum wire, the wave function $\phi(n^{(e)}, m^{(e)}, \boldsymbol{\rho})$ has the form:

$$\phi(n^{(e)}, m^{(e)}, \boldsymbol{\rho}) = J_{m^{(e)}}\left[\mu_{n^{(e)}}(m^{(e)})\frac{\rho}{\rho_0}\right], \tag{28}$$

where $\mu_{n^{(e)}}(m^{(e)})$ is $n^{(e)}$-th root of $m^{(e)}$-th order Bessel function, $\chi(n^{(e)}, m^{(e)}, z)$ is the wave function which may be obtained after solving the self-consistent problem. Thus, the total wave function from Eq. (27) must be normalized.

Generally, the value of polaron binding energy $\Delta E_{pol,wire}$ is determined by the optical phonon spectrum properties and depends on electron size-quantization level number. It is necessary to take into account the optical phonons localized both inside the quantum wire and at the hetero-interface. We obtain this energy after the angle averaging procedure expressible in explicit form:

$$\Delta E_{pol,wire} = -\sum_{n,q}\frac{\alpha^2(0, n, q)}{\hbar\omega_0} - \sum_{q}\frac{\alpha^2(0, q)}{\hbar\omega_S}. \tag{29}$$

Here $\alpha(0, n, q)$ and $\alpha(0, q)$ are the coefficients defined in Eq. (6). The value of $\Delta E_{pol,wire}$ from Eq. (29) is defined by the interaction of an electron with phonon modes for which $m = 0$ and contains the contribution caused by interaction with both confined and interface phonons for all size-quantization levels. Eq. (29) can be used for numerical analysis of electron-phonon interaction characteristic properties for the quantum wires of various symmetry. At the same time, the electron energy and wave function are obtained analytically when the inequality from Eq. (26) is satisfied.

The interaction of an electron with interface phonon mode of the frequency close to barrier frequency $\omega_{LO}^{(b)}$ gives the most significant contribution to the polaron binding energy in the parameter Eq. (26). It has the form:

$$\Delta E_{pol,wire} = \frac{e^2}{2\varepsilon_{opt}^{(b)}}\sum_{q}\left|\int|\chi(z)|^2\exp[iqz]dz\right|^2\ln(q\rho_0). \tag{30}$$

Eq. (30) contains the optical dielectric function of the barriers $\varepsilon_{opt}^{(b)}$. In other words, the polaron states arise independently of the quantum wire material dielectric properties. Contribution due to these properties can be obtained in higher orders in the parameter from Eq. (26). It can be seen from Eq. (30) that phonon wave vector q characteristic values that determine the electron-phonon interaction are inversely proportional to the polaron radius magnitude, that is $q \simeq 1/a_0$. In this region, the logarithmic function changes slightly, and we can obtain the energy $\Delta E_{pol,wire}$ with the same accuracy in parameter from Eq. (26):

$$\Delta E_{pol,wire} = \frac{e^2}{2\,\varepsilon_{opt}^{(b)}} \ln\left(\frac{\rho_0}{a_0}\right) \sum_{q} \left| \int |\chi(z)|^2 \exp\left[iqz\right] dz \right|^2. \tag{31}$$

The electron polaron binding energy as the functional of unknown yet wave function $\chi(z)$ can be obtained by substituting Eq. (31) into the average Hamiltonian from Eq. (4) and by variational method:

$$-\frac{\hbar^2}{2\,m_e}\frac{d^2\chi(z)}{dz} - \left(\frac{e^2}{\varepsilon_{opt}^{(b)}} \ln\left(\frac{a_0}{\rho_0}\right)\right) \chi^3(z) = E_{pol}^{(e)}\,\chi(z). \tag{32}$$

The solution of nonlinear Eq. (32) has the form:

$$\chi(z) = \frac{1}{\sqrt{2\,a_0}} \frac{1}{ch(z/a_0)}. \tag{33}$$

By substituting the wave function from Eq. (33) into Eq. (32), we obtain the polaron binding energy as:

$$E_{pol,wire}^{(e)} = -\frac{Me^4}{\hbar^2\left(\varepsilon_{opt}^{(b)}\right)^2} \ln^2\left(\frac{a_0}{\rho_0}\right). \tag{34}$$

Thus, the polaron radius a_0 contains the adiabatic parameter from Eq. (25) and is equal to:

$$a_0 = \frac{\hbar^2\,\varepsilon_{opt}^{(b)}}{m_e\,e^2 \ln\left(\frac{a_0}{\rho_0}\right)}. \tag{35}$$

The substitution of the material parameters [18] for *ZnSe*/*CdSe*/*ZnSe* quantum wire into Eq. (35) leads one to expect that the strong polaron effects should be observed at a wire radius $\rho_0 < 40\ \mathring{A}$.

The condition for polaron exciton appearance in a quantum wire is analogous to that considered above for a quantum well, Eq. (18). The basic requirement is a significant difference between the hole and the electron masses. If the radius of a quantum wire corresponds to the conditions from Eqs. (21) and (22), a complete compensation of the contributions from the electron and hole does not occur, and a strong electron-phonon interaction is possible.

4. Spherical quantum dot

In this chapter, we study the structures in which the quantum dot and matrix materials have different phonon modes and its dielectric functions are described by Eq. (10). We have used the approximation presented in [19], where the interface phonon spectrum is described by the following equation:

$$l\,\varepsilon^{(d)}(\omega) + (l+1)\,\varepsilon^{(m)}(\omega) = 0, \tag{36}$$

where $\varepsilon^{(d)}(\omega)$ and $\varepsilon^{(m)}(\omega)$ are the dielectric functions of the quantum dot and matrix materials, respectively; l is the number of the spherical harmonic for corresponding interface vibration. If $l = 0$, there is only one solution, which coincides with ω_{LO} in the matrix material. For $l \neq 0$, there are two solutions for the interface phonon frequencies.

For our problem, the coefficients $\alpha(r, n)$ from Eq. (6) have the form [19]:

$$\alpha(v, nlm) = \hbar\,\omega_{LO}^{(m)}\,\rho(nlm)\left(\frac{4\pi e^2}{r_0\,\mu_{nl}^2\,j_{l+1}^2(\mu_{nl})\,\varepsilon_{opt}^{(m)}}\right)^{1/2} \tag{37}$$

for the bulk phonons and

$$\alpha(s, l) = -\left(\frac{2\pi e^2}{\omega^2 r_0}\right)^{1/2}\left[\varepsilon_{\infty}^{(d)}\frac{\omega_{LO,d}^2-\omega_{TO,d}^2}{\left(\omega^2-\omega_{TO,d}^2\right)^2}\,l+\varepsilon_{\infty}^{(d)}\frac{\omega_{LO,m}^2-\omega_{TO,m}^2}{\left(\omega^2-\omega_{TO,m}^2\right)^2}(l+1)\right]^{-1/2}\cdot\hbar\,\omega_s\,\rho_s(lm) \tag{38}$$

for the interface phonons. Here r_0 is the quantum dot radius; j_l are the spherical Bessel functions; and $j_l(\mu_{nl}) = 0$. The quantities $\rho(nlm)$ and $\rho_s(lm)$ are the bulk and interface phonons densities, respectively, which have the form:

$$\rho(nlm) = j_l\left(\mu_{nl}\frac{r}{r_0}\right)Y_{lm}(\theta,\phi), \tag{39}$$

$$\rho_s(lm) = \left(\frac{r}{r_0}\right)^l Y_{lm}(\theta,\phi), \tag{40}$$

where $Y_{lm}(\theta, \phi)$ are the spherical wave functions. After the averaging procedure over the electron wave function $\Psi(\mathbf{r})$, the values of the densities from the equations should be replaced by its average values:

$$\rho_{av} = \int d^3 r\,|\Psi(\mathbf{r})|^2\,\rho(nlm), \tag{41}$$

$$\rho_{s,av} = \int d^3 r\,|\Psi(\mathbf{r})|^2\,\rho_s(lm). \tag{42}$$

In this case, the energy of electron size quantization level polaron shift has the form:

$$\Delta E_{pol,dot} = -\sum_{n,l,m}\hbar\,\omega_{LO}\,|\alpha(v, nl)|^2\,|\rho_{av}|^2-\sum_{l,m}\hbar\omega(l)\,|\alpha(s, l)|^2\,|\rho_{s,av}|^2. \tag{43}$$

As follows from Eq. (43), the bulk and interface phonon contributions to the polaron binding energy are summed. It will be seen from the further consideration that the interface phonon contribution can exceed the surface phonon one under certain conditions. The results obtained make it possible to calculate the polaron shifts for any size quantization level. Consider a polaron shift for a particle with a spherical wave function. For example, it could be an electron in the ground state. The polaron shift can be obtained analytically [20] and is equal to:

$$E_{pol,dot}^{(e)} = -\frac{e^2}{r_0}\left(\frac{0.39}{\varepsilon_{opt}^{(d)}} + \frac{0.5}{\varepsilon_{opt}^{(m)}}\right). \tag{44}$$

It follows from Eq. (44) that taking into account matrix polarization leads to an increase in the polaron effect. It should be noted that there is a noticeable polaron shift even for quantum dots based on a nonpolar material. This is due to the presence of interface phonons that create the polarization in surrounding matrix. Note also that for the quantum dot case, the contributions of charged particle interaction with bulk and interface phonons are of the same order of magnitude in the adiabatic parameter.

$$r_0 \ll a_0. \tag{45}$$

This is the main difference between this problem and the quantum well and quantum wire considered earlier. For these structures, the largest contribution in the adiabatic parameters from Eq. (11) and Eq. (25) is caused by the interface phonons. The inequality (45) is satisfied, for example, for *CdSe* quantum dots in a *ZnSe* matrix when the dot radius $r_0 < 30\ \mathring{A}$.

Another significant feature of the polaron in quantum dots is a significant suppression of the polaron exciton state. The exciton polaron shift turns out to be zero for the localization of the electron and hole with wave functions of the same symmetry inside the quantum dot. The nonzero interaction of an exciton with polar optical phonons arises for different symmetries of the electron and hole wave functions only. This is possible if the quantum dot is made of a material where interband transitions are forbidden (e.g., CuO_2) or if the valence band complex spectrum is taken into account. The latter is typical for most III–V and II–VI semiconductor compounds. It is shown in [20] that taking into account the valence band degeneracy in the Luttinger Hamiltonian model leads to a noticeable difference between the polaron shift for the electron and hole. In this case, the exciton-phonon interaction can turn out to be strong at the quantum dot.

5. Weak electron: phonon interaction

The interaction of charge particles with polar optical phonons can be weak in nanostructures based on materials with low ionicity. When the condition Eq. (3) is satisfied, the electron-phonon interaction described by the Hamiltonian $\hat{H}_{e-ph}$ can be taken into account by the perturbation theory [21]. In the bulk crystals with weak electron-phonon interaction, the position of the ground electronic state level is shifted, and the electron effective mass increases [22]. Our calculations have shown that similar effects arise in a quantum well, and they are mainly due to the interaction of charge carriers with interface optical phonons. The level position displacement corresponds to the renormalization of the forbidden band width. When the electron-phonon interaction is weak, this effect is rather small. Therefore, the main attention will focus to polaron effect on the charged carrier effective mass change. This change for an electron depends on the material dielectric properties of both the quantum well and barriers. A quasi-two-dimensional analog of known results for bulk materials [22] is obtained in the sufficiently narrow quantum well for which the size quantization energy ΔE_m exceeds the quantum well localized optical phonon energy $\hbar\omega^{(w)}(\mathbf{q})$ and interface optical phonon energy

$\hbar\omega^{(s)}(\mathbf{q})$. The main contribution to the electron ground state energy correction with respect to parameter $\Delta E_m/\hbar\omega^{(w)}(\mathbf{q})$ has the form:

$$\Delta E_m = \frac{\pi}{2}\alpha_{eff}\hbar\omega^{(b)} + \frac{p^2}{2m^*}. \tag{46}$$

The frequency from Eq. (46) is $\omega^{(b)} = \omega^{(s)}(0)$. The polaron mass is equal to:

$$m_{pol} = \frac{m^{(w)}}{1 - \pi\alpha_{eff}/8}. \tag{47}$$

Eqs. (46) and (47) are similar to the known results from two-dimensional polaron theory [14]. However, the effective coupling constant is equal to:

$$\alpha_{eff} = \frac{e^2}{2\hbar\omega^{(b)}}\left(\frac{2m^{(w)}\omega^{(b)}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty^{(b)}} - \frac{1}{\varepsilon_0^{(b)}}\right). \tag{48}$$

It is seen from Eq. (48) that, just as in the case of a strong-coupling polaron, the effective electron-phonon interaction constant is determined by the effective electron mass inside the quantum well and the barrier material dielectric properties. This value is analogous to the Frohlich constant, but it is not a characteristic of any particular material and is determined by the quantum well properties. In a specific approximation, when the condition $q \ll 1/L$ is satisfied, the charge particle interaction with polar optical phonons is defined by the interface phonon spectrum. The interface phonon frequencies in the same approximation are close to ones for the barrier optical phonons and can differ markedly from the quantum well optical phonon frequencies. This may explain the discrepancy between the experimental and theoretical values of the effective polaron mass for the *ZnO-ZnMgO* quantum well, obtained in [23]. In estimating the effective mass, the authors of [23] have used the Frohlich constant for *ZnO* instead of the effective constant from Eq. (48). Using the effective constants of Eq. (48) greatly improves the agreement between theory and experimental data.

6. Conclusions

It is shown that the interface phonons play an important role in the polaron state formation in quantum nanostructures. In quantum wells and quantum wires, the polaron binding energy is determined mainly by the interaction of charged particles with interface optical phonons. In the quantum dots, the contribution due to the interaction with interface phonons is additive with the energy of interaction with bulk phonons. Moreover, for nanostructures based on the same materials, the polaron binding energy increases with the structure dimensionality reduction.

Thus, the results obtained show that the barrier material ionicity degree plays a fundamental role for forming the large radius polarons in quantum wells and quantum wires. Meanwhile, the quantum well itself can be based on low ionicity material. The interaction of charged particles with interface optical phonons is the reason that the polaron effects are enhanced significantly.

The condition for observing a polaron exciton is the essential difference between the electron and hole effective masses. In this case, only partial compensation of the phonon interaction with charged particles occurs, and the achievement of a strong electron-phonon interaction is possible.

Thus, the appearance of strong polaron effects is a clear demonstration of the interface phonon influence on optical and transport properties of nanostructures.

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