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Interface Phonons and Polaron Effect in Quantum Wires

A. Yu. Maslov · O. V. Proshina

Abstract The theory of large radius polaron in the quantum wire is developed. The interaction of charge particles with interface optical phonons as well as with optical phonons localized in the quantum wire is taken into account. The interface phonon contribution is shown to be dominant for narrow quantum wires. The wave functions and polaron binding energy are found. It is determined that polaron binding energy depends on the electron mass inside the wire and on the polarization properties of the barrier material.

Keywords Quantum wire · Electron–phonon interaction · Interface phonons · Polaron

Introduction

The electron–phonon interaction in semiconductor heterostructures is of greater interest in comparison to bulk materials. This is due to the fact that the quasi-particle space localization leads to the modifications of the energy spectrum. The all-important factor is the rise of new vibration branches of optical spectrum, namely, the interface optical phonon [1]. In addition, the intensity of electron–phonon interaction is changed. The interaction of charge particles with polar optical phonons should exhibit the most intensity. This interaction is of considerable importance in the understanding of the properties of heterostructures based on material with high ionicity. It can lead to self-consistent bond state of a charge particle and phonons, that is, the large radius polaron [2].

Currently, an investigation on the part played by interface phonons has attracted considerable interest in polaron state formation study. The heterostructures of different symmetry are under investigation. The contributions to polaron binding energy both of interface and of bulk optical phonons are the same value order in the quantum dots [3–5]. Taking into account, interface phonons are essential for quantitative analysis of the polaron states. It does not lead to new qualitative effects. Alternatively, the interface phonon role dominates in polaron binding energy for quantum well case [6, 7]. In response to this fact, the strong electron–phonon interaction can be realized in the quantum wells based on non-polar material with high iconicity barrier material. In addition, from the results, it follows that profound polaron effects should be expected, e.g., in the Si/SiO_2 compounds. Although there are no polar optical phonons in the material of such quantum well, these may be produced at the heteroboundary. As a result, the strong interaction of charged particles with interface phonons becomes possible. Conversely, the essential depression of electron–phonon interaction is possible when the quantum well is made of polar material and for the barriers is taken non-polar material.

In recent years, varied technologies of semiconductor quantum wire growth with assorted barriers are progressing rapidly. The most success has been achieved for the quantum wires based on III–V compounds [8–12]. Some advances have been made in the formation of II–VI semiconductor wire structures [13, 14]. It is in these structures that the polaron states can arise. At the same time, no extended theoretical study of the polaron states in such structures is available. Proper allowance must be made for the interaction of charge particles with interface optical

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phonons for an understanding of this problem. In this paper, we develop a theory of polarons in the quantum wires, taking into account the interaction of charged particles with all branches of the optical phonon spectrum.

Interface Phonons in the Quantum Wire

The interface phonon spectrum is being examined in [15]. The general equations have been obtained to describe the phonon spectrum taking into account the interaction of polarization and deformation potentials. In materials with high ionicity degree, the charge particle interaction with polar optical phonons is of crucial importance in polaron state formation. This has led us to use the model which takes into account this phonon type in the quantum wire. The polar optical phonons we describe by the outline suggested in [16]. Optical-phonon modes in the quantum wire are determined using the classical electrostatics equations:

$$\mathbf{P}(\mathbf{r}) = \chi_i(\omega)\mathbf{E}(\mathbf{r}), \tag{1a}$$

$$E(r) = -\nabla\varphi(r), \tag{1b}$$

$$\nabla^2\varphi(\mathbf{r}) = -4\pi\rho(\mathbf{r}), \tag{1c}$$

$$\rho(\mathbf{r}) = -\nabla\mathbf{P}(\mathbf{r}), \tag{1d}$$

together with conventional boundary conditions at heterointerfaces, where $\mathbf{P}(\mathbf{r})$ is the polarization field, $\mathbf{E}(\mathbf{r})$ the electric field, $\varphi(\mathbf{r})$ the scalar potential, $\rho(\mathbf{r})$ the total charge density, and $\chi^{(i)}(\omega)$ is the dielectric susceptibility of the material i ($i = 1, 2$). The dielectric function $\varepsilon^{(i)}(\omega)$ is given by:

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

where $\omega_{LO}^{(i)}$ and $\omega_{TO}^{(i)}$ are the frequencies of longitudinal-optical (LO) phonons and transverse-optical (TO) phonons, respectively, and $\varepsilon_\infty^{(i)}$ is the high-frequency dielectric constant. The solution of system (Eq. 1) for the cylindrical quantum wire leads to the equation defining the dispersion law for interface optical phonons:

$$\frac{I'_m(k\rho_0)}{I_m(k\rho_0)}\varepsilon^{(1)}(\omega) = \frac{K'_m(k\rho_0)}{K_m(k\rho_0)}\varepsilon^{(2)}(\omega). \tag{3}$$

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, k is the wave vector, ρ_0 is the quantum wire radius. The spectrum of interface phonons is determined by solution of Eq. 3. In Fig. 1 is shown the wave-vector dependence of the interface phonon frequencies. This dependence is calculated for the quantum wire based on CdSe surrounded by ZnSe barriers with $m = 0$ in Eq. 3. The material parameters are taken from [17].
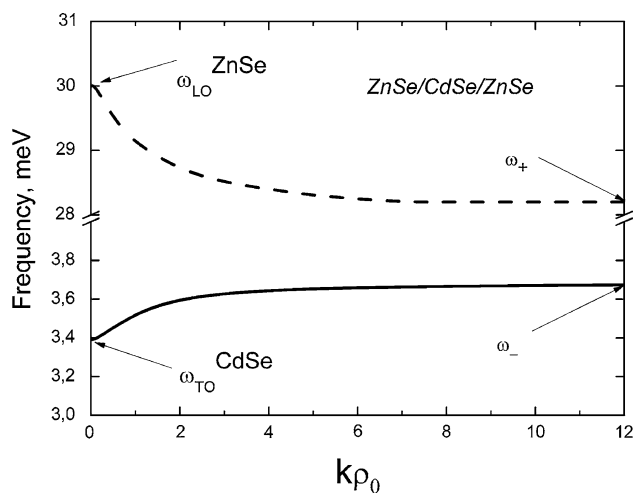

Fig. 1 The wave-vector dependence of interface optical phonon frequencies for *ZnSe/CdSe/ZnSe* quantum wire

The Hamiltonian operator for phonon subsystem is conveniently written in terms of the phonon creation and annihilation operators:

$$\widehat{H}_{ph} = \sum_{k,n,m}\hbar\omega_0 a_{nm}^+(k)a_{nm}(k) + \sum_{k,m}\hbar\omega_m(k)a_{mk}^+ a_{mk}, \tag{4}$$

where the operators $a_{nm}^+(k)$ describe the creation of bulk phonons localized inside the quantum wire, a_{mk}^+ are the interface phonon creation operators. The Hamiltonian of electron–phonon interaction for the cylindrical quantum wire can be represented by the method supposed in [16]:

$$\widehat{H}_{e-ph} = \sum_{k,m,n}\alpha_{mn}(k,\boldsymbol{\rho})\big[a_{nm}(k) + a_{nm}^+(k)\big]$$
$$+ \sum_{k,m}\alpha_m(k)\big[a_{mk}^+ + a_{mk}\big]. \tag{5}$$

Here, the coefficients $\alpha_{mn}(k,\boldsymbol{\rho})$ are defined as:

$$\alpha_{mn}(k,\boldsymbol{\rho}) = \left(\frac{2\pi e^2\hbar\omega_{LO}}{L}\right)^{1/2}$$
$$\times \frac{1}{\left(\varepsilon_{opt}^{(1)}\right)^{1/2}\rho_0}\frac{\exp[ikz]J_m(k\rho)\exp[im\varphi]}{\left(q^2 + \frac{1}{\rho_0^2}\mu_n^2(m)\right)^{1/2}}; \rho \le \rho_0, \tag{6}$$

here, $\mu_n(m)$ is n-th order root of the equation $J_m(\mu) = 0$, J_m is the m-th order Bessel function of the first kind. The interaction parameters $\alpha_m(k)$ have the form:

$$\alpha_m(k) = \left(\frac{2\pi\omega_s e^2}{L}\right)^{1/2}$$
$$\times \left[\beta_{(1)}^{-1}(\omega_s)I_1(k\rho_0) + \beta_{(2)}^{-1}(\omega_s)\frac{I_m(k\rho_0)}{K_m(k\rho_0)}I_2(k\rho_0)\right]^{1/2} \times$$
$$\frac{I_m(k\rho)}{I_m(k\rho_0)}\exp[im\varphi]\exp[ikz]; \rho \le \rho_0 \tag{7}$$

The expressions (6), (7) do not require in the region $\rho \ge \rho_0$.

The reason is that we suppose the total electron localization within the quantum wire. In Eq. 7 were used the following symbols:

$$\beta(\omega) = \frac{1}{\varepsilon_{opt}} \frac{\omega_{LO}^2}{\omega^2} \left(\frac{\omega^2 - \omega_{TO}^2}{\omega_{LO}^2 - \omega_{TO}^2} \right)^2, \tag{8}$$

$$I_1(k\rho_0) = \int\limits_0^{k\rho_0} \left[I_m^2(z) + \left(\frac{dI_m(z)}{dz} \right)^2 + \frac{m^2}{z^2} I_m^2(z) \right] z\,dz, \tag{9}$$

$$I_2(k\rho_0) = \int\limits_{k\rho_0}^\infty \left[K_m^2(z) + \left(\frac{dK_m(z)}{dz} \right)^2 + \frac{m^2}{z^2} K_m^2(z) \right] z\,dz. \tag{10}$$

The Polaron in the Quantum Wire

We consider a cylindrical quantum wire with the radius ρ_0. Let the quantum wire be surrounded with compositionally identical barriers. In order to separate the effect of exactly dielectric irregularities, we assume that the potential well for electrons is rather deep, so that the penetration of the wave functions under the barrier can be disregarded. In this case, the interaction of charged particles with barrier phonons is weak. We write the Hamiltonian of the system as

$$\widehat{H} = \widehat{H}_e + \widehat{H}_{ph} + \widehat{H}_{e-ph} \tag{11}$$

Here, $\widehat{H}_e$ is the electron Hamiltonian for which the interaction of the electron with phonons is disregarded. The Hamiltonian is given by

$$\widehat{H}_e = -\frac{\hbar^2}{2M} \nabla^2 + V(\boldsymbol{\rho}) \tag{12}$$

where $V(\boldsymbol{\rho})$ is the quantum wire potential and M is the electron effective mass. If the interaction of an electron with polar optical phonons is strong, the polaron binding energy can be determined with the use of adiabatic approximation. In so doing, the electron subsystem is fast and phonon subsystem is slow. The adiabatic parameter here is the ratio of the quantum wire radius ρ_0 to the polaron radius a_0:

$$\frac{\rho_0}{a_0} \ll 1. \tag{13}$$

The exact expression for polaron radius a_0 is obtained below. The condition (Eq. 13) implies that the main contribution to the polaron binding energy is given by small values of the wave vector k such that

$$k\rho_0 < 1. \tag{14}$$

If condition (Eq. 13) is satisfied, the wave function of an electron localized in the n-th size-quantization level can be represented as:

$$\Psi_e(\mathbf{r}) = \varphi(n^{(e)}, m^{(e)}, \boldsymbol{\rho}) \exp\left[im^{(e)} \varphi \right] \chi\left(n^{(e)}, m^{(e)}, z \right), \tag{15}$$

where the wave function $\varphi(n^{(e)}, m^{(e)}, \boldsymbol{\rho})$ describes the two-dimensional electron motion not disturbed by electron–phonon interaction. This motion occurs inside the quantum wire. The wave function $\chi(n^{(e)}, m^{(e)}, z)$ represents the electron localization in the self-consistent potential well created by phonons. The quantum numbers $n^{(e)}$, $m^{(e)}$ define not disturbed electron state in the quantum wire. In the case of total electron localization in the cylindrical quantum wire, the wave function $\varphi(n^{(e)}, m^{(e)}, \boldsymbol{\rho})$ has the form:

$$\varphi(n^{(e)}, m^{(e)}, \boldsymbol{\rho}) = J_{m^{(e)}} \left[\mu_{n^{(e)}} \left(m^{(e)} \right) \frac{\rho}{\rho_0} \right]. \tag{16}$$

Here $\mu_{n^{(e)}}(m^{(e)})$ is $n^{(e)}$-th root of $m^{(e)}$-th order Bessel function. The wave function $\chi(n^{(e)}, m^{(e)}, z)$ is to be obtained by solving self-consistent problem. In so doing, the total wave function from Eq. 15 is perceived to be normalized.

The procedure of polaron binding energy determination is similar to that used in [7]. We average the total Hamiltonian of the system from expression (Eq. 11) with yet unknown electron wave function from formula (Eq. 15). The Hamiltonian $\widehat{H}_e$ from (Eq. 12) takes the form after this procedure:

$$\left\langle \widehat{H}_e \right\rangle = E_{n^{(e)}, m^{(e)}}^{(0)} + \frac{\hbar^2}{2M} \int dz \left(\frac{d\chi(z)}{dz} \right)^2. \tag{17}$$

Here $E_{n^{(e)}, m^{(e)}}^{(0)}$ is the energy of an electron on relevant size-quantization level, M is the electron mass inside the quantum wire. The form of phonon Hamiltonian $\widehat{H}_{ph}$ from Eq. 11 remains unchanged. Averaged Hamiltonian of electron–phonon interaction $\widehat{H}_{e-ph}$ can be written as:

$$\left\langle \widehat{H}_{e-ph} \right\rangle = \sum_{k,m,n} \widetilde{\alpha}_{mn}(k) \left[a_{nm}(k) + a_{nm}^+(k) \right]$$
$$+ \sum_{k,m} \widetilde{\alpha}_m(k) \left[a_{mk} + a_{mk}^+ \right]. \tag{18}$$

Here, $\widetilde{\alpha}_{mn}(k)$ and $\widetilde{\alpha}_m(k)$ are the coefficients $\alpha_{mn}(k, \boldsymbol{\rho})$ and $\alpha_m(k)$ from Eq. 5 averaged with the electron wave function from formula (Eq. 15). We obtain average Hamiltonian $\widehat{H}_{av}$:

$$\widehat{H}_{av} = \widehat{H}_{ph} + \left\langle \widehat{H}_{e-ph} \right\rangle. \tag{19}$$

It can be brought to the form diagonal in phonon variables by the unitary transformation $e^{-U} \widehat{H}_{av} e^U$, where

$$U = \sum_{k,m,n} \widetilde{\alpha}_{mn}(k) \left[a_{nm}(k) - a_{nm}^+(k) \right]$$
$$+ \sum_{k,m} \widetilde{\alpha}_m(k) \left[a_{mk} - a_{mk}^+ \right]. \tag{20}$$

The unitary transformation application gives the following equation:

$$e^{-U}\widehat{H}_{av}e^{U} = \widehat{H}_{ph} + \Delta E_e \qquad (21)$$

From expression (Eq. 21), we can see that, in the adiabatic approximation used here, the bulk phonon spectrum and the interface phonon spectrum remain unchanged. The last summand in expression (Eq. 21) presents the energy of a large radius polaron. In the general case, the energy ΔE_e involved in (Eq. 21) depends on the dielectric properties of the materials of both the quantum wire and the barriers. In the general case, the polaron binding energy ΔE_e depends on electron size-quantization level number and on optical-phonon spectrum properties. These phonons are localized in the quantum wire and at the heteroboundary. After the procedure of angle averaging which is expressible in explicit form, we obtain this energy ΔE_e as:

$$\Delta E_e = -\sum_{n,k} \frac{\widetilde{\alpha}^2(0,n,k)}{\hbar\omega_0} - \sum_k \frac{\widetilde{\alpha}^2(0,k)}{\hbar\omega_S}. \qquad (22)$$

The energy (Eq. 22) is defined by the electron interaction with phonon modes correspond to $m = 0$ only. This equation (Eq. 22) contains the contribution to polaron energy for all size-quantization levels. This contribution is caused by the interaction of localized electron with confined and interface phonons. It can be used for numerical analysis of electron–phonon interaction characteristic properties. However, the electron energy and wave function can be obtained analytically on condition the unequality (Eq. 14) is satisfied.

Results and Discussion

The most significant contribution to the polaron binding energy in the parameter (Eq. 14) gives the interaction of an electron with interface phonon mode of the frequency close to barrier frequency $\omega_{LO}^{(2)}$. The largest contribution to the energy in the parameter (Eq. 14) has the form:

$$\Delta E_e = \frac{e^2}{2\varepsilon_{opt}^{(2)}} \sum_k \left| \int |\chi(z)|^2 \exp[ikz]dz \right|^2 \ln(k\rho_0). \qquad (23)$$

The Eq. 23 contains the optical dielectric function of the barriers $\varepsilon_{opt}^{(2)}$. It is defined as $\frac{1}{\varepsilon_{opt}} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}$. This quantity comes about from taking into account the interaction of an electron with interface optical phonons. It is seen from Eq. 23 that the quantum wire material properties have no effect on the polaron state formation. The part of quantum wire material dielectric properties can be obtained in higher orders in the parameter (Eq. 14). It is seen from Eq. 23 that the characteristic values of the phonon wave vector k which describe the value of electron–phonon interaction is of the order reciprocal to polaron radius a_0 $\left(k \sim a_0^{-1}\right)$. The logarithmic function changes weakly in this region.

Therefore, we can consider with the same accuracy in parameter (14) that the energy is equal to:

$$\Delta E_e = \frac{e^2}{2\varepsilon_{opt}^{(2)}} \ln\left(\frac{\rho_0}{a_0}\right) \sum_k \left| \int |\chi(z)|^2 \exp[ikz]dz \right|^2 \qquad (24)$$

The substitution of the energy from Eq. 24 to the average Hamiltonian from Eq. 19 leads to the expression for polaron binding energy as the functional of unknown yet wave function $\chi(z)$. It can be written as:

$$E_{pol} = \frac{\hbar^2}{2M} \int \left(\frac{d\chi(z)}{dz}\right)^2 dz + \frac{e^2}{2\varepsilon_{opt}^{(2)}} \ln\left(\frac{\rho_0}{a_0}\right)$$
$$\times \sum_k \left| \int |\chi(z)|^2 \exp[ikz]dz \right|^2. \qquad (25)$$

The following equation is obtained by variational method using wave functions $\chi(z)$:

$$-\frac{\hbar^2}{2M}\frac{d^2\chi(z)}{dz} - \left(\frac{e^2}{\varepsilon_{opt}^{(2)}} \ln\left(\frac{a_0}{\rho_0}\right)\right)\chi^3(z) = E_{pol}\chi(z). \qquad (26)$$

This nonlinear Eq. 26 has the solutions which can be written in the form with any energy values E_{pol}:

$$\chi(z) = \frac{1}{\sqrt{2a_0}} \frac{1}{ch(z/a_0)}. \qquad (27)$$

The polaron binding energy is found by substitution of Eq. 27 to 26:

$$E_{pol} = -\frac{Me^4}{\hbar^2 \left(\varepsilon_{opt}^{(2)}\right)^2} \ln^2\left(\frac{a_0}{\rho_0}\right). \qquad (28)$$

The polaron radius a_0 is obtained by solving the transcendental equation. It has the form:

$$a_0 = \frac{\hbar^2 \varepsilon_{opt}^{(2)}}{Me^2 \ln\left(\frac{a_0}{\rho_0}\right)}. \qquad (29)$$

It is this quantity from Eq. 29 which contains the adiabatic parameter (Eq. 13). Substituting material parameters [17] into Eq. 29 for the quantum wire ZnSe/CdSe/ZnSe leads one to expect that the strong polaron effects for these structure should be observed when the quantum wire radius $\rho_0 < 40\ \mathring{A}$.

It might be well to point out that both the polaron binding energy (Eq. 28) and polaron radius (Eq. 29) depend on effective electron mass inside the quantum wire and barrier dielectric properties. This clearly demonstrates the prevailing role of the interaction of an electron with interface optical phonons. The availability of the surface phonons leads to widening the range of materials in which the strong polaron effect should be expected. The strong electron–phonon interaction may exist near the interface

between polar and non-polar materials. Among other things the significant electron–phonon interaction can result from the interface phonon influence in Si/SiO$_2$ heterostructures.

The results obtained show that the intensity of electron–phonon interaction is determined significantly by interface optical phonons in narrow quantum wires corresponding to the condition (Eq. 13). These interface phonons are localized basically in the heteroboundary vicinity. And its field penetrates also into the barriers region. By this is meant that the interface phonons can produce the effective canal of excitation transfer in the structures with several quantum wires. Related ways should be allowed for the transport theory development in quantum nanostructures.

References

1. P. Halevi, *Electromagnetic surface modes* (Wiley, New York, 1982)
2. I.P. Ipatova, A.Yu. Maslov, O.V. Proshina, Surf. Sci. **507–510**, 598 (2002)
3. D.V. Melnikov, W.B. Fowler, Phys. Rev. B **64**, 245320 (2001)
4. A.L. Vartanian, A.I. Asatryan, A.A. Kirakosyan, J. Phys. Cond. Mater. **14**, 13357 (2002)
5. A.Yu. Maslov, O.V. Proshina, A.N. Rusina, Semiconductors **41**, 822 (2007)
6. A.Yu. Maslov, O.V. Proshina, Superlattices Microstruct. **47**, 369 (2010)
7. A.Yu. Maslov, O.V. Proshina, Semiconductors **44**, 189 (2010)
8. Zh.M. Wang, Sh Seydmohamadi, V.R. Yazdanpanah, G.J. Salamo, Phys. Rev. B **71**, 165309 (2005)
9. X. Wang, Zh.M. Wang, B. Liang, G.J. Salamo, Ch.-K. Shih, Nano Letters **6**, 1847 (2006)
10. J. Lee, Zh. Wang, B. Liang, W. Black, V.P. Kunets, Y. Mazur, G.J. Salamo, Ieee Trans. Nanotechnol. **6**, 70 (2007)
11. J.B. Schlager, K.A. Bertness, P.T. Blanchard, L.H. Robins, A. Roshko, N.A. Sanford, J. Appl. Phys. **103**, 124309 (2008)
12. M. Jeppsson, K.A. Dick, J.B. Wagner, P. Caroff, K. Deppert, L. Samuelson, L.-E. Wernersson, J. Crystal. Growth **310**, 4115 (2008)
13. B. Zhang, W. Wang, T. Yasuda, Y. Li, Y. Segawa, H. Yaguchi, K. Onabe, K. Edamatsu, T. Itoh, Ipn. J. Appl. Phys. **36**, L1490 (1997)
14. L. Chen, P.J. Klar, W. Heimbrodt, F.J. Brieler, M. Fröba, H.-A. Krug von Nidda, T. Kurz, A. Loidl, J. Appl. Phys. **93**, 1326 (2003)
15. C. Trallero-Giner, Physica. Scripta. **55**, 50 (1994)
16. M. Mori, T. Ando, Phys. Rev. B **40**, 6175 (1989)
17. Landolt-Bornstein, *Numerical data and functional relationships in science and technology, v. 17b* (Springer, Berlin, 1982)