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Unusual Properties of Interface Phonons in Quantum Wells Based on Uniaxial Materials

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Abstract
The spectrum of interface phonons is studied theoretically for quantum wells made by using uniaxial materials. It is shown that the spectrum features provide information on anisotropy degree of both the quantum well and barrier materials. The special properties of charge particle interaction with interface optical phonons are predicted. It was found that the interaction is suppressed when the barrier material has strongly anisotropic dielectric properties. In the case of weak anisotropy, the interaction is suppressed only at small and very large values of the phonon wave vector. However, there is a region of intermediate values of wave vectors in which strong electron-phonon interaction is possible. This can lead to the appearance of large-radius polarons. The features of such polarons differ from those of the excitations studied earlier. The results obtained expand the possibilities of optical diagnostics of the quantum nanostructures.
Keywords: *Quantum well, Electron-phonon interaction, Polaron, Uniaxial symmetry materials, Interface optical phonons.*

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I. INTRODUCTION

The interaction of charged particles with polar optical phonons can be quite significant in high ionicity materials where the electron-phonon interaction constant may exceed the unity. In addition, the appearance of new elementary excitations, that are the bound states of charged particles and polar optical phonons, may happen even in bulk materials. These are the large-radius polarons [1]. The conditions for polaron creation are most favorable for the quantum-dimensional structures. The additional branches of polar optical phonons, namely interface phonons, appear in such structures. The manifestation of polaron effects on optical spectra is a clear demonstration of the interface phonon influence on optical and transport properties of nanostructures. Besides, the effective electron-phonon interaction increases with decreasing the structure dimensionality. The polaron creation significantly changes the optical and transport properties of the quantum wells, wires and dots. We are aware of the publications in which theoretical studies of large radius polaron in nano-heterostructures take into consideration the interaction with only one polar phonon mode [2–5]. This description seems to us insufficient. Changes in the phonon spectrum of nanostructures can be very significant. To describe adequately the polaron states, it is necessary to take into account the interaction of charge particles with all phonon branches of the spectrum.

II. RESULTS AND DISCUSSION

In this paper the theory of charged particle interaction with interface optical phonons is developed for quantum wells based on uniaxial symmetry materials. In order to compare the results obtained, we start with the problem of polarons in quantum wells based on the cubic symmetry materials. To understand the role of interaction with the branches of interface phonons consider the case of complete localization of the electron within a quantum well. In this case, the interaction of the electron with phonons of barrier material may be neglected. But at the same time, the barrier effect is very important. It is determined by the structure and features of interface phonon spectrum. To determine the properties of interface phonons, we apply the continuum model proposed in [6]. The spectrum of the symmetric mode of interface phonons is determined from the solution of the following equation:

$$\varepsilon^{well}(\omega) th\left(\frac{ql}{2}\right) + \varepsilon^{bar}(\omega) = 0 \ . \qquad (1)$$

Here l is the quantum well characteristic size, q is two-dimensional wave vector. $\varepsilon^{well}(\omega)$, $\varepsilon^{bar}(\omega)$ are the dielectric functions of the quantum well and barriers, respectively. The dielectric function in the region of phonon frequencies is defined by the expression:

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

where ω_{LO}, ω_{TO} are the frequencies of longitudinal and transverse optical phonons, respectively ε_∞ is the high-frequency dielectric constant. The equation Eq. (2) means that the approximation of dispersion less modes for bulk optical phonons has been used. In this approximation interface and bulk phonon modes we can consider independently [7,8]. The contributions of interface phonon antisymmetric modes vanish when the Hamiltonian is averaged over the wave function of an electron localized in a symmetric quantum well. The amplification of the electron-phonon interaction occurs in fairly narrow quantum wells having a width *l* that is less than the polaron radius ρ_0:

$$l < \rho_0 . \tag{3}$$

It is this quantity from Eq. (3) on which the adiabatic approximation is based. If the inequality (3) holds, the electron wave function $\Psi_m^{el}(\mathbf{r})$ can be represented as a product:

$$\Psi_m^{el}(\mathbf{r}) = \varphi_m(z)\chi_m(\mathbf{r}_l), \tag{4}$$

Here $\varphi_m(z)$ is the wave function of transverse motion which is determined by the quantum well potential, $\mathbf{r}_l$ is the two–dimensional plane well coordinate, $\chi_m(\mathbf{r}_l)$ is the two-dimensional wave function which is determined by electron localization in a self-consistent quantum well created by polar optical phonons.

The polaron binding energy in the quantum well we have obtained in [8]. It has the form:

$$E_{pol}^{el} = -0.4 \frac{m_e e^4}{\left(\varepsilon_{opt}^{bar}\right)^2 \hbar^2}, \tag{5}$$

where ε_{opt}^{bar} from expression $\frac{1}{\varepsilon_{opt}^{bar}} = \frac{1}{\varepsilon_\infty^{bar}} - \frac{1}{\varepsilon_0^{bar}}$ is the optical dielectric function of the barrier material.

Some corrections to the polaron binding energy (5) can be obtained if we take the next order in the parameter (3). We get:

$$\Delta E_{pol} = 0.07 E_{pol}^{el} \frac{l}{\rho_0^{el}} (D_V + D_S), \tag{6}$$

The dimensionless parameters D_V and D_S are determined by the complex combinations of the phonon frequencies in the quantum well and barrier materials and are found in [8]. It turns out that the corrections to the polaron binding energy are related to the interaction with both bulk and interface phonons. These corrections may have different signs [8]. The value of total binding energy depends essentially on the dielectric properties of both the quantum well and the barrier materials. The main contribution to the polaron binding energy coincides with our result obtained in [9] by dint of approximate method for the phonon field calculations. But it is impossible to accurately incorporate the corrections using this method. To define the quantity ΔE_{pol} from Eq. (6) we should take into consideration the quantum well phonon spectrum.

The electron polaron radius ρ_0^{el} turns out to be equal to:

$$\rho_0^{el} = \frac{\hbar^2 \varepsilon_{opt}^{bar}}{m_e e^2}. \tag{7}$$

A similar analysis can be carried out for the hole polaron. By analogy with Eq. (5), the main contribution to its binding energy is written as:

$$E_{pol}^{h} = -0.4 \frac{m_h e^4}{\hbar^2 \left(\varepsilon_{opt}^{bar}\right)^2}. \tag{8}$$

For most semiconductors the hole mass m_h is much larger than the electron one m_{el}. Consequently, the binding energy of the hole polaron from Eq. (8) is much larger than the value obtained from Eq. (5). And the region of localization for the hole polaron ρ_0^h is smaller than that for the electron polaron ρ_0^{el}:

$$\rho_0^h = \frac{m_{el}}{m_h} \rho_0^{el} << \rho_0^{el}. \tag{9}$$

The inequality (9) plays an important role in the polaron exciton theory. The exciton interaction with optical phonons has a number of specific features. The electron and hole create the medium polarization which compensates each other partially. This compensation essentially depends on the ratio of the electron ρ_0^{el}, hole ρ_0^{h} and exciton ρ_0^{ex} polaron radii. The influence of the barrier dielectric properties on the exciton state here must be taken into consideration for narrow quantum well case.

The main contribution to polaron exciton binding energy is caused by the hole localization in the polaron potential well and is determined by hole polaron radius ρ_0^{h}. The polarization pruduced by the electron compensates partially the hole polarization. The radius of quasi-two-dimensional exciton ρ_0^{ex} similar to Eq.(7) and with considering Eq. (9) has the form:

$$\rho_0^{ex} = \frac{\hbar^2 \varepsilon_0^{bar}}{\mu e^2}, \tag{10}$$

where μ is the electron – hole reduced mass. It is seen from (7), (9) and (10) that the electron polaron radius always exceeds the exciton one: $\rho_0^{el} > \rho_0^{ex}$. If the inequality $\rho_0^{h} > \rho_0^{ex}$ holds, the polarizations created by the electron and by the hole are compensated. Usually in this situation the condition of strong coupling exciton with phonons is not implemented.

In the opposite case when

$$\rho_0^{h} < \rho_0^{ex}, \tag{11}$$

the strong exciton-phonon interaction can be realized.

Taking into consideration Eq. (11) and only main contributions to the parameter from Eq. (3), one can obtain the polaron exciton binding energy as:

$$E_{ex} = 0.4 \frac{m_h e^4}{\hbar^2 \left(\varepsilon_{opt}^{bar}\right)^2} - 2 \frac{m_{el} e^4}{\hbar^2 \left(\varepsilon_{\infty}^{bar}\right)^2}. \tag{12}$$

Compared to the first one, the second term in Eq. (12) is small in parameter $m_{el} / m_h \ll 1$. We can see from Eq. (12) that the strong coupling possibility for the exciton and optical phonons depends on parameters of both the quantum well and barrier materials. The polaron exciton formation requires a significant difference between the electron and hole effective masses in the quantum well. Moreover, the barriers must be made of high ionicity materials. If so, the polarization properties of the quantum well material do not play a significant role.

The heterovalent II-VI/III-V quantum wells are more promising target for the experimental study of polaron effects in the case of strong electron-phonon interaction. The growth technologies have been developing successfully in recent times [10]. In quantum wells produced using II-VI compounds, the interaction of charged particles and excitons with optical phonons can be strong. In the III-V compounds, the effective masses of the carriers within the quantum well are small. The barrier optical dielectric function for II-VI materials is also rather small. The values of the polaron and exciton radii in quantum wells can increase by a factor of two to three compared with them for II-VI compounds. The exciton radius ρ_0^{ex} from Eq. (10) is in the range $50 \div 100$ *Å*. The electron polaron radius ρ_0^{el} from Eq. (7) falls within the range $70 \div 200$ *Å* and hole polaron one ρ_0^{h} from Eq. (9) is approximately $20 \div 50$ *Å*. Thereby, a quasi-two-dimensional polaron in heterovalent quantum wells can be observed for the well widths $l \leq 50$ *Å*. Quantum wells of more complex configuration (for example, I-VII/III-V) can also become a promising object for the polaron effect study provided if the strong electron-phonon interaction takes place.

In our previous articles [8, 11] we looked at the problems when both the quantum well and barriers are made of cubic symmetry materials. Many of hetero-structures based on II–VI compounds which have lower symmetry, for example, hexagonal. This may dramatically change the character of the phonon spectrum. Therefore, the results obtained in the framework of the cubic approximation turn out to be inapplicable. So, the application of the cubic approximation to ZnO/ZnMgO quantum well [12] led to substantial discrepancy between the theoretical estimates and the experimental data.

Let us now consider what will change for quantum wells based on materials with uniaxial symmetry. In this case, the optical axis of the hexagonal material is directed perpendicular to the quantum well plane. Such nanostructures are currently being investigated experimentally [13, 14]. In these structures, the conditions of strong electron-phonon interaction can be realized.

The interface optical phonon spectrum can be found using the procedure proposed in [6]. In the region of phonon frequencies, the dielectric function of the crystal is represented by Eq.(2). For uniaxial materials in

the chosen geometry, the dielectric tensor has a diagonal form. In this case, the *xy* plane coincides with the quantum well plane and $\varepsilon_{xx}(\omega) = \varepsilon_{yy}(\omega) = \varepsilon_t(\omega)$. The direction of the *z*-axis coincides with the optical axis one and for it $\varepsilon_{zz}(\omega) = \varepsilon_l(\omega) \neq \varepsilon_t(\omega)$. When both the quantum well and the barriers, which are assumed to be symmetric, are made of uniaxial materials, then, taking into account (1), we obtain equations for the spectrum of interface phonons for the symmetric mode in the following form:

$$\varepsilon_l^{bar}(\omega)\beta^{bar}(\omega) = -\varepsilon_l^{well}(\omega)\beta^{well}(\omega)th\left(\frac{qa}{2}\beta^{well}(\omega)\right). \quad (13)$$

For the antisymmetric mode we obtain:

$$\varepsilon_l^{bar}(\omega)\beta^{bar}(\omega) = -\varepsilon_l^{well}(\omega)\beta^{well}(\omega)cth\left(\frac{qa}{2}\beta^{well}(\omega)\right). \quad (14)$$

The dimensionless coefficients $\beta^{bar}(\omega)$, $\beta^{well}(\omega)$ are equal to $\beta^{bar}(\omega) = \sqrt{\varepsilon_t^{bar}(\omega)/\varepsilon_l^{bar}(\omega)}$ and $\beta^{well}(\omega) = \sqrt{\varepsilon_t^{well}(\omega)/\varepsilon_l^{well}(\omega)}$ and vary from zero to infinity.

The equations (13) and (14) have solutions in the frequency ranges where $\varepsilon_t^{bar}(\omega)$ and $\varepsilon_t^{well}(\omega)$ have different signs, and pairs of quantities $\varepsilon_t^{bar}(\omega)$, $\varepsilon_l^{bar}(\omega)$ and $\varepsilon_t^{well}(\omega)$, $\varepsilon_l^{well}(\omega)$ have the same signs. In the general case, there are two solutions for each of equations (13) and (14) that satisfy these conditions. For definiteness, we will assume that the following relations hold in both the well and the barriers: $\omega_{LO,t} > \omega_{LO,l}$ and $\omega_{TO,t} > \omega_{TO,l}$. We assume that the phonon frequencies of the materials of quantum well and barriers do not overlap. In this case, Eqs. (13) and (14) have the following pairs of solutions. The first of them turns out to be in the region of the phonon frequencies of the barriers. Accordingly, the second pair of solutions turns out to be in the region of phonon frequencies of the quantum well material.

In the situation where the well (or barriers) are made of materials of cubic symmetry, Eqs. (13) and (14) are somewhat simplified. In this case, it is necessary to substitute to these expressions $\beta^{bar}(\omega) = \beta^{well}(\omega) = 1$.

The spectrum of interface optical phonons is shown in Figure 1 for the case of weak phonon anisotropy. For the dependences shown in the figure, the following model frequency ratios were used in the calculations: $\omega_{TO,t} = 1.05\omega_{TO,l}$; $\omega_{LO,l} = 1.8\ \omega_{TO,l}$; $\omega_{LO,t} = 1.85\omega_{TO,l}$.

For the case of strong phonon anisotropy, the spectrum of interface phonons is shown in Figure 2 and the frequency ratios are $\omega_{TO,t} = 1.35\omega_{TO,l}$; $\omega_{LO,l} = 1.6\ \omega_{TO,l}$; $\omega_{LO,t} = 1.8\omega_{TO,l}$. In Figure 1 and Figure 2, for comparison, the dashed lines represent the spectrum in the cubic approximation when $\beta^{bar}(\omega) = \beta^{well}(\omega) = 1$ and the average frequency values were used for the materials of the quantum well and barriers.

Note that the ranges of possible values of the interface phonon frequencies turned out to be somewhat narrower than in the case of heterostructures based on cubic materials. The use of the cubic approximation for any method of averaging phonon frequencies gives not quite accurate results even for the spectrum of interface phonons. These discrepancies increase with an increase in the degree of phonon anisotropy of the materials used. Thus, the study of the spectrum of interface phonons makes it possible to independently determine the dielectric parameters of bulk materials used in the quantum well fabrication.

The differences between the quantum wells based on cubic and hexagonal materials turn out to be more significant when studying the electron-phonon interaction.

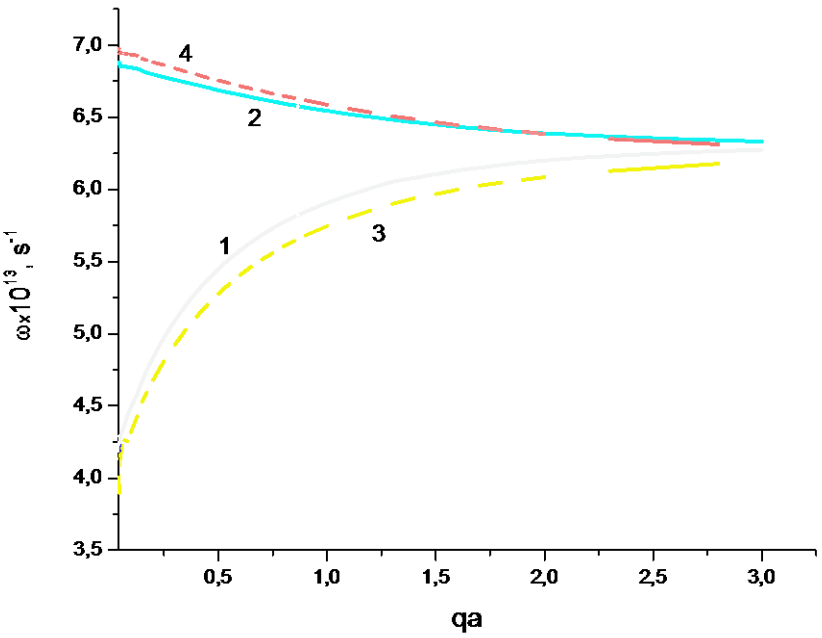

Figure 1: Spectrum of Interface Phonons in the Case of Weak Phonon Anisotropy. 1 -symmetric, 2 - antisymmetric mode for uniaxial material; 3 - symmetric, 4 - antisymmetric mode for cubic material.

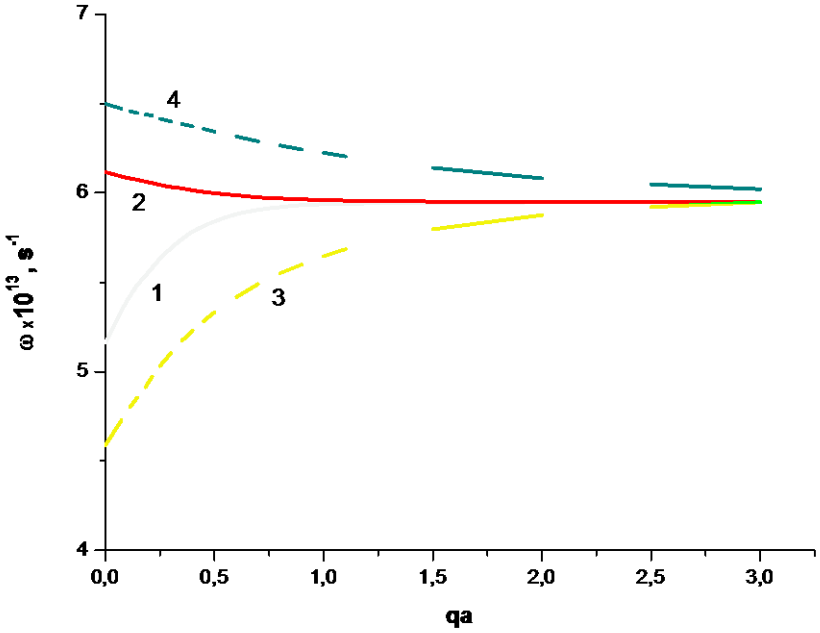

Figure 2: Spectrum of Interface Phonons in the Case of Strong Phonon Anisotropy. 1 -symmetric, 2 - antisymmetric mode for uniaxial material; 3 - symmetric, 4 - antisymmetric mode for cubic material.

The potential of electron-phonon interaction is obtained according to the scheme proposed in [6], taking into account the lower symmetry of the dielectric constant of the materials of the well and barriers. The coefficients $\beta^{bar}(\omega)$ and $\beta^{well}(\omega)$ included in the expression for the electron-phonon interaction, which we do not present here because of its bulkiness, vary from zero to infinity with, as a rule, a small change in frequencies (from $\omega_{LO,l}^{bar}$ to $\omega_{LO,t}^{bar}$ and in other similar frequency intervals). Therefore, the frequency dependence for the

parameters of the electron-phonon interaction turns out to be very strong. The presence of even a small anisotropy leads to the qualitative change in the nature of the electron-phonon interaction. It turns out that the most significant effect is associated with the anisotropy of the barrier material.

Two qualitatively different situations can be distinguished, depending on the ratio of the parameters determining the dielectric anisotropy of the barriers. To estimate the measure of anisotropy, it is convenient to take a parameter *b* equal to

$$b = \frac{\left|\omega_{LO,l}^2 - \omega_{LO,t}^2\right|}{\omega_{LO,l}^2}. \qquad (15)$$

The interaction of charged particles with interface optical phonons turns out to be weak if the parameter *b* is large enough (of the order of unity). According to Figure 2, the spectrum of interface phonons differs greatly from the results obtained in the cubic approximation. In this case, the electron-phonon interaction can be taken into account according to the perturbation theory. The formation of the large-radius polarons does not occur in this situation. To take into account the electron–phonon interaction correctly, in addition to the interface phonons, it is also necessary to take into account other types of excitations, namely, phonons localized in the quantum well [15] and extraordinary phonons [16].

We have another case for weak anisotropy of the phonon spectrum, when the parameter *b* from expression (15) turns out to be small ($b \ll 1$). For the majority of II-VI compounds, this value of the parameter b is realized. In this case, there is an interval of values of the phonon wave vector $\mathbf{q}$, in which

$$b \ll qa < 1. \qquad (16)$$

In such interval, the interaction of charged particles with interface optical phonons turns out to be parametrically large in comparison with the interaction with other branches of the phonon spectrum. When Eq. (16) is satisfied, the main contribution to the electron-phonon interaction is reduced to the two-dimensional interaction of the Frohlich type, with the interaction constant equal to

$$A_F = \frac{e^2}{2\hbar\omega^{bar}}\left(\frac{2m^{well}\omega^{bar}}{\hbar}\right)^{1/2}\frac{1}{\varepsilon_{opt}^{bar}}. \qquad (17)$$

The difference between the longitudinal and transverse parameters of the barriers can be neglected here. It should be noted that the effective coupling constant A_F depends on both the parameters of the quantum well and the barriers. Therefore, it turns out to be a characteristic of the structure, and not of any one specific material. The main difference of these structures from those fabricated using materials of cubic symmetry is that the region of existence of Frohlich-type interaction is limited in terms of the wave vector values, not only from above but also from below. The strong electron-phonon interaction is possible at $A_F > 1$ and weak one if $A_F < 1$ is realized. In the case of the strong interaction, large-radius polarons should appear in the quantum well, which represent the bound state of a charged particle and interface optical phonons. The radius of the polaron state is defined by Eqs.(7,9). We emphasize that *m* is the mass of charge particle within the quantum well. The appearance of polaron states in the structure is possible only if the polaron radius ρ_0 satisfies the relation in which the condition from Eq. (16) is taken into account:

$$b \ll \frac{a}{\rho_0} < 1. \qquad (18)$$

III. CONCLUSIONS

It was shown that the interaction of charge particles with interface optical phonons depends on the phonon spectrum anisotropy. With strong anisotropy degree, the interaction turns out to be significantly less than one in similar structures made of cubic symmetry materials. In the case of weak phonon anisotropy, conditions are found under which the interaction of charged particles with optical phonons can be described by the coupling constant of the Fröhlich type. It turns out that both weak and strong electron-phonon interaction can be realized in various structures. Our results expand the possibilities for optical diagnostics of quantum nanostructures by non-destructive optical methods. The results obtained also demonstrate that the study of interface optical phonon spectrum allows us to determine the parameters of bulk materials used in the nanostructure fabrication.

REFERENCES

[1]. Alexandrov A.S., Devreese J.T. (2010) "Advances in Polaron Physics" (Berlin Heidelberg Springer-Verlag) 165 p.
[2]. Pokatilov E.P., Klimin S.W., Fomin V.M., Devreese J.T., Wise F.M. (2002) "Multiphonon Raman scattering in semiconductor nanocrystals: Importance of Nonadiabatic Transitions" Phys. Rev. B, Vol. 65, Pp. 075316.

[3]. Yeranosyan M.A., Vartanian A.L., Vardanyan K.A. (2016) "Influence of Spin–Orbit Interactions on the Polaron Properties in Wurtzite Semiconductor Quantum Well" Physica E: Low-Dim Sys., Vol. 75, Pp. 330-335.
[4]. Miyata K., Meggiolaro D., Trinh M.T., Joshi P.P., Mosconi E., Jones S.C., De Angelis F., Zhu X.-Y. (2017) "Large Polarons in Lead Halide Perovskites" Science Advances, Vol. 3, Pp. e1701217.
[5]. Vartanian A., Kirakosyan A., Vardanyan K. (2017) "Fröhlich polaron in Nanowire with Rashba and Dresselhaus Spin-Orbit Couplings" Superlattices and Microstructures, Vol. 109, Pp 655-661.
[6]. Mori M., Ando T. (1989) "Electron–Optical Phonon Interaction in Single and Double Heterostructures" Phys. Rev. B, Vol. 40, Pp. 6175.
[7]. Ridley B.K. (2017) "Hybrid Phonons in Nanostructures" (Oxford, New York:Oxford University Press) 192 p.
[8]. Maslov A.Yu., Proshina O.V. (2010) "The Role of Interface Phonons in the Formation of Polaron States in Quantum Wells" Semiconductors" Vol. 44, Pp. 189–193.
[9]. Maslov A.Yu., Proshina O.V., Rusina A.N. (2009) "Interface Phonon Effect on Optical Spectra of Quantum Nanostructures" J. Luminesc., Vol. 129, Pp. 1934-1936.
[10]. Lassise M.B., Wang P., Tracy B.D., Chen G., Smith D.J., Zhang Y.H. (2018) "Growth of II-VI/III-V Heterovalent Quantum Structures" Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics, Vol. 36, Pp. 02D110.
[11]. Maslov A.Yu., Proshina O.V. (2015) "Polaron Mass of Charge Carriers in Semiconductor Quantum Wells" Semiconductors, Vol. 49, Pp. 1344-1347.
[12]. Imanaka Y., Takamasu T., Tampo H., Shibata H., Niki S. (2010) "Two-Dimensional Polaron Mass in ZnO Quantum Hall Systems" Phys. Stat. Solidi C, Vol. 7, Pp. 1599-1601.
[13]. Lopez-Ponce M., Nakamura A., Suzuki M., Temmyo J., Agouram S., Martínez-Tomás M.C., Muñoz-Sanjosé V., Lefebvre P., Ulloa J.M., Muñoz E., Hierro A. (2014) "VIS-UV ZnCdO/ZnO Multiple Quantum Well Nanowires and the Quantification of Cd Diffusion" Nanotechnology, Vol. 25, Pp. 255202.
[14]. Sun C.Q. (2020) "Electron and Phonon Spectrometrics" (Springer Nature, Singapur) 517 p.
[15]. Wang Z., Reinhardt K., Dutta M., Stroscio M.A. (2014) in "Length-Scale Dependent Phonon Interactions" Eds: Shindé S.L., Srivastava G.P. (Springer Science+Business Media, New York, USA), Ch. 2.
[16]. Maslov A.Yu., Proshina O.V. (2018) "Extraordinary phonons in II-VI quantum wells" Int. J. Mech. Eng. Technol., Vol. 9, No 13, Pp. 1653-1659.