# Electron–optical-phonon interaction in quantum wells consisting of mixed crystals

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A theory of electron–optical-phonon interactions in quantum wells consisting of mixed crystals is reported. According to whether the well or the barrier is made of mixed crystals, quantum wells consisting of mixed crystals are divided into three types. The expressions of phonon frequencies of all phonon modes and the electron–LO-phonon interaction Hamiltonian of all the types of the quantum wells are obtained based on the dielectric continuum approach. As applications of the present theory, the concentration dependences and the dispersion relations of the interface-optical-phonon frequencies in $GaAs/Ga_xAl_{1-x}As$, $Zn_xCd_{1-x}Se/ZnSe$, and $ZnS_xSe_{1-x}/ZnS$ quantum wells are calculated. The interaction energies of an electron in the lowest subband state with every optical phonon mode are also calculated. The features of the polaronic effect in quantum wells consisting of mixed crystals are discussed. [S0163-1829(99)01431-9]

## I. INTRODUCTION

In the past two decades, electronic and optical properties of quasi-two-dimensional structures, such as quantum wells (QW's) and heterojunctions, have attracted much attention. Since the electron-phonon interaction plays a dominant role for many of these properties, it has been a subject of intense study in recent years. Based on the dielectric continuum model,[1] many authors studied electron-phonon interactions for various layered structures.[2–6] Polaronic effects on electrons and excitons in QW's were also studied extensively.[7–16]

Although most experiments have been carried out in QW's consisting of mixed crystals, but, to the best of our knowledge, effects of the mixed crystal on the polaronic properties in the quantum wells have not been investigated up to now. Almost all the published works assumed the layered structures are composed of binary crystals or used the effective phonon approximation for ternary mixed crystals.[17] In fact, it is well known that there are two LO- and two TO-phonon modes in a ternary mixed crystal theoretically. According to the oscillator strengths and the features of the modes, mixed crystals are classed into ''one-mode'' and ''two-mode'' behavior types. In a ''one-mode'' mixed crystal, the oscillator strengths remain approximately constant and one of the oscillator strengths of the two LO (TO) modes is much larger than the other. Furthermore, the frequency ($k\sim 0$) of the stronger mode varies approximately linearly with concentration from the frequency characteristic of one end member to that of the other end member. In this case, only the stronger mode must be considered actually in the study and the application of the mixed crystal. For a ''two-mode'' crystal, the two LO- (TO-) phonon frequencies are observed to occur at frequencies close to those of the end members of the ternary mixed crystal. Furthermore, the oscillator strengths of the two LO (TO) modes vary approximately proportionally to the mole fraction of the component it represents. The criteria for the one-mode and two-mode behavior of mixed crystals were discussed in detail by many authors.[18–20] The properties of mixed crystals are very different from the binary crystals and will greatly affect the optical and electronic properties of QW's consisting of mixed crystals. The features of the electron-phonon interaction in QW's consisting of mixed crystals must be studied.

Very recently we have investigated the phonon mode and the electron-phonon interaction in ternary mixed crystals based on the pseudo-unit-cell approximation.[21] In the present paper we extend our previous work and give a theoretical study of the problem of phonon modes and electron-phonon interaction in QW's consisting of mixed crystals. The expressions of phonon frequencies and the electron–LO-phonon interaction Hamiltonian of the QW's are obtained by using the dielectric continuum approach. On the basis of the present work, many theoretical investigations can be done in more detail. As applications, the concentration dependence and the dispersion relations of the interface-optical- (IO) phonon frequencies, the polaron energies of some typical quantum wells are calculated. We want to answer the questions of how many phonon modes there are in the QW's and how much the multiphonon-mode property of mixed crystals affects the polaronic effect in the QW consisting of mixed crystals.

The theoretical method and the procedure used in this paper were described in detail by Wendler and Pechstedt (Ref. 3) and Mori and Ando (Ref. 5); here we do not rewrite it again in detail and show our results directly with a brief necessary explanation.

## II. PHONON MODE AND PHONON FREQUENCY

We consider a sandwich structure which involves layers of mixed materials. The $z$ axis is chosen perpendicular to the heterointerfaces. The well layer (denoted as 1) is in the region of $|z|\leqslant d$, and made of one polar semiconductor with

 

TABLE I. Number of phonon mode, phonon frequency, or phonon frequency equation in QW's.

| QW | Phonon mode | $j$ | Frequency or phonon frequency equation |
|---|---|---|---|
| | Confined LO | 1 | $\omega_{L1}$ |
| | Half-space LO | $2a,2b$ | $\omega_{L2a},\ \omega_{L2b}$ |
| $TBT$ | Symmetric IO | 1,2,3 | $\epsilon_2^+\frac{(\omega_{L2a}^2-\omega^2)(\omega_{L2b}^2-\omega^2)}{(\omega_{T2a}^2-\omega^2)(\omega_{T2b}^2-\omega^2)}+\epsilon_1^+\frac{(\omega_{L1}^2-\omega^2)}{(\omega_{T1}^2-\omega^2)}=0$ |
| | Antisymmetric IO | 1,2,3 | $\epsilon_2^-\frac{(\omega_{L2a}^2-\omega^2)(\omega_{L2b}^2-\omega^2)}{(\omega_{T2a}^2-\omega^2)(\omega_{T2b}^2-\omega^2)}+\epsilon_1^-\frac{(\omega_{L1}^2-\omega^2)}{(\omega_{T1}^2-\omega^2)}=0$ |
| | Confined LO | $1a,1b$ | $\omega_{L1a},\omega_{L1b}$ |
| | Half-space LO | 1 | $\omega_{L2}$ |
| $BTB$ | Symmetric IO | 1,2,3 | $\epsilon_2^+\frac{(\omega_{L2}^2-\omega^2)}{(\omega_{T2}^2-\omega^2)}+\epsilon_1^+\frac{(\omega_{L1a}^2-\omega^2)(\omega_{L1b}^2-\omega^2)}{(\omega_{T1a}^2-\omega^2)(\omega_{T1b}^2-\omega^2)}=0$ |
| | Antisymmetric IO | 1,2,3 | $\epsilon_2^-\frac{(\omega_{L2}^2-\omega^2)}{(\omega_{T2}^2-\omega^2)}+\epsilon_1^-\frac{(\omega_{L1a}^2-\omega^2)(\omega_{L1b}^2-\omega^2)}{(\omega_{T1a}^2-\omega^2)(\omega_{T1b}^2-\omega^2)}=0$ |
| | Confined LO | $1a,1b$ | $\omega_{L1a},\ \omega_{L1b}$ |
| | Half-space LO | $2a,2b$ | $\omega_{L2a},\ \omega_{L2b}$ |
| $TTT$ | Symmetric IO | 1,2,3,4 | $\epsilon_2^+\frac{(\omega_{L2a}^2-\omega^2)(\omega_{L2b}^2-\omega^2)}{(\omega_{T2a}^2-\omega^2)(\omega_{T2b}^2-\omega^2)}+\epsilon_1^+\frac{(\omega_{L1a}^2-\omega^2)(\omega_{L1b}^2-\omega^2)}{(\omega_{T1a}^2-\omega^2)(\omega_{T1b}^2-\omega^2)}=0$ |
| | Antisymmetric IO | 1,2,3,4 | $\epsilon_2^-\frac{(\omega_{L2a}^2-\omega^2)(\omega_{L2b}^2-\omega^2)}{(\omega_{T2a}^2-\omega^2)(\omega_{T2b}^2-\omega^2)}+\epsilon_1^-\frac{(\omega_{L1a}^2-\omega^2)(\omega_{L1b}^2-\omega^2)}{(\omega_{T1a}^2-\omega^2)(\omega_{T1b}^2-\omega^2)}=0$ |

dielectric function $\epsilon_1(\omega)$. The two barrier layers in the region of $z>d$ and $z<-d$ are made of another polar semiconductor (denoted as 2) with dielectric function $\epsilon_2(\omega)$. Each dielectric function is assumed to be isotropic and independent of wave vector. In this paper, we take three types of QW's into consideration. (I) The well is made of a binary crystal and the barrier of a ternary mixed crystal. This type of QW is denoted as a $TBT$-type QW. (II) The well is made of a ternary mixed crystal and the barrier of a binary crystal. This type of QW is denoted as a $BTB$-type QW. (III) The well is made of a ternary mixed crystal and the barrier of another ternary mixed crystal. This type of QW is denoted as a $TTT$-type QW. It is well known that the dielectric functions of a binary crystal and a ternary mixed crystal are taken in the forms of

$$\epsilon_i(\omega)=\epsilon_{\infty i}\frac{(\omega^2-\omega_{Li}^2)}{(\omega^2-\omega_{Ti}^2)}, \tag{2.1}$$

and

$$\epsilon_i(\omega)=\epsilon_{\infty i}\frac{(\omega^2-\omega_{Lia}^2)(\omega^2-\omega_{Lib}^2)}{(\omega^2-\omega_{Tia}^2)(\omega^2-\omega_{Tib}^2)}, \tag{2.2}$$

respectively, where $i$ corresponds to the material 1 or 2. $\omega_{Li}$ ($\omega_{Ti}$) is the longitudinal (transverse) optical-phonon frequency of the binary crystal. $\omega_{Lia}$ and $\omega_{Lib}$ ($\omega_{Tia}$ and $\omega_{Tib}$) are the two longitudinal (transverse) optical-phonon frequencies of the ternary mixed crystal. $\epsilon_{\infty i}$ ($\epsilon_{0i}$) is the optical (static) dielectric constant of the material indicated by $i$.

Setting $\Phi(\mathbf{r},t)$ denotes the scalar potential of the LO phonon, then the electric field resulting from the LO phonon is given by $\mathbf{E}(\mathbf{r},t)=-\boldsymbol{\nabla}\Phi(\mathbf{r},t)$. Because of the translational invariance along the interface, we can introduce two-dimensional (2D) Fourier transforms along the $x$-$y$ plane and work in $(\mathbf{k},z)$ space, where $\mathbf{k}$ is a 2D wave vector. No net charge resides in either material, so that we get the wave equation of the LO-phonon modes in each layer from Maxwell's equations:

$$\epsilon_i(\omega)\left(\frac{\partial^2}{\partial z^2}-k^2\right)\Phi(\mathbf{k},z)=0. \tag{2.3}$$

This equation is the main equation determining phonon modes. The electromagnetic boundary conditions are $\Phi(\mathbf{r},t)$ and $\epsilon_i(\omega)\partial\Phi(\mathbf{r},t)/\partial z$ are continuous across the interfaces at $z=d$ and $z=-d$. The phonon frequency and dispersion relations of phonons in QW's can be determined analytically from Eq. (2.3) and the boundary condition. Amplitudes of phonon eigenmodes are determined by the orthonormalization condition. The $\epsilon_i(\omega)=0$ case yields bulklike-type phonons. Frequencies of the bulklike phonons, i.e., confined LO-phonon mode for $|z|\leqslant d$ and half-space LO-phonon mode for $|z|>d$, are independent of the wave vector and are given directly by the bulk LO-phonon frequencies. For the $\epsilon_i(\omega)\neq 0$ case, $(\partial^2/\partial z^2-k^2)\Phi(\mathbf{k},z)=0$ holds and the solution of this equation with the boundary condition mentioned above yields IO-phonon modes and dispersion relations of the IO-phonon modes. The results are listed in Table I. In this table $\epsilon_1^{\pm}$ and $\epsilon_2^{\pm}$ are defined by

$$\epsilon_1^{\pm}=\epsilon_{\infty 1}(1\mp e^{-2kd}), \tag{2.4}$$

$$\epsilon_2^{\pm}=\epsilon_{\infty 2}(1\pm e^{-2kd}). \tag{2.5}$$

The present theory shows that the pictures of the phonon modes in the QW's composed of mixed crystals are very different from the effective phonon approximation.[8,9] From Table I we know the following: (1) In the *TBT* QW, there are two half-space LO-phonon modes, one slab LO-phonon mode, three symmetric and three antisymmetric IO-phonon modes; (2) in the *BTB* QW, there are one half-space LO-phonon mode, two slab LO-phonon modes, three symmetric and three antisymmetric IO-phonon modes; and (3) in the *TTT* QW, there are two half-space LO-phonon modes, two slab LO-phonon modes, and four symmetric and four antisymmetric IO-phonon modes.

## III. ELECTRON-PHONON INTERACTION HAMILTONIAN

If one obtains the complete set of eigenfunctions of Eq. (2.3) with the boundary condition, then the interaction energy of an electron (charge $-e$) at the position $\mathbf{r}$ with polarizable medium is given by $H_i=-e\Phi(\mathbf{r},t)$. The electron–LO-phonon interaction Hamiltonian in a QW takes the form of

$$H_i=\sum_{\beta}\sum_{\mathbf{k}}[V_{k\beta}L_{k\beta}(z)\exp(i\mathbf{k}\cdot\boldsymbol{\rho})a_{\mathbf{k}\beta}+\text{H.c.}], \tag{3.1}$$

where $a_{\mathbf{k}\beta}(a^{\dagger}_{\mathbf{k}\beta})$ is the annihilation (creation) operator of an optical phonon with frequency $\omega_{\beta}(\mathbf{k})$ and wave vector $(\mathbf{k},k_{\beta})$. $\beta=jm$ refers to the confined LO phonon in the well with frequency $\omega_{Lj}$ and wave vector $k_m=m\pi/2d$, where $j=1$ corresponds to a binary crystal and $j=1a,1b$ to a ternary crystal. The positive integer $m$ is limited by the Brillouin-zone boundary, that is, $m_{\max}=\text{int}(2d/a)$. $a$ is the lattice constant of the well material. $\beta=jk_z$ refers to the half-space LO phonon in the barrier with frequency $\omega_{Lj}$ and wave vector $k_z$. $j=2$ denotes a binary crystal, and $j=2a,2b$ a ternary mixed crystal. Finally, $\beta=+j$ refers to symmetric IO-phonon modes, and $\beta=-j$ to antisymmetric IO-phonon modes. $j$ $(=1,2,\ldots)$ denotes the number of the IO-phonon modes. $\mathbf{r}=(\boldsymbol{\rho},z)$ is the position of the electron, and $\boldsymbol{\rho}$ is a two-dimensional vector in the $x$-$y$ plane.

TABLE II. $L_{k\beta}(z)$ in a QW.

| Phonon mode | $L_{k\beta}(z)$ | Region |
|---|---|---|
| Confined LO | $\sin[k_m(z+d)]$ | $\lvert z\rvert\leqslant d$ |
| Half-space LO | $\sin[k_z(\lvert z\rvert-d)]$ | $\lvert z\rvert>d$ |
| | $\exp[-k(z-d)]$ | $z>d$ |
| Symmetric IO | $\cosh(kz)/\cosh(kd)$ | $\lvert z\rvert\leqslant d$ |
| | $\exp[k(z+d)]$ | $z<-d$ |
| | $\exp[-k(z-d)]$ | $z>d$ |
| Antisymmetric IO | $\sinh(kz)/\sinh(kd)$ | $\lvert z\rvert\leqslant d$ |
| | $-\exp[k(z+d)]$ | $z<-d$ |

$L_{k\beta}(z)$ is an eigenfunction of Eq. (2.3). Fourier constant $V_{k\beta}$ represents the strength of electron-phonon coupling, which is determined by the orthonormalization condition of phonon modes. By a lengthy analytical calculation, $L_{k\beta}(z)$ and $V_{k\beta}$ of all the phonon modes are obtained and listed in Tables II and III, respectively. In Table III some abbreviations are defined by

$$\frac{1}{=\epsilon_i}=\left(\frac{1}{\epsilon_{\infty i}}-\frac{1}{\epsilon_{0i}}\right)\quad(i=1,2), \tag{3.2}$$

$$\frac{1}{=\epsilon_{i\pm j}(\omega)}=\left(\frac{1}{\epsilon_{\infty i}}-\frac{1}{\epsilon_{0i}}\right)\left(\frac{\omega_{\pm j}^2-\omega_{Ti}^2}{\omega_{Li}^2-\omega_{Ti}^2}\,\frac{\omega_{Li}}{\omega_{\pm j}}\right)^2$$

$$(i=1,2;\ \ j=1,2,\ldots). \tag{3.3}$$

$\bar{\epsilon}_{ij}(\omega_{Lj})$ is the effective dielectric constant of the mixed crystal in the well ($i=1$ and $j=1a,1b$) or in the barrier ($i=2$ and $j=2a,2b$), $\bar{\epsilon}_{ij}(\omega_{\pm j})$ is the effective dielectric constant corresponding to the IO-phonon mode in mixed crystal in the well ($i=1$) or the barrier ($i=2$). The two effective dielectric constants can be defined in one form of

$$\bar{\epsilon}_{ij}(\omega)=\frac{[\epsilon_i(\omega)+2-a_i(x_i)]^2\omega^2}{a_i^2(x_i)\{x_i\omega_{i1T}[\sqrt{\tilde{\epsilon}_{i01}-\tilde{\epsilon}_{i\infty 1}}/(\tilde{\epsilon}_{i\infty 1}+2)]\sqrt{\mu_{i1}/m_{ij}(\omega)}C_{ij}(\omega)+(1-x_i)\omega_{i2T}[\sqrt{\tilde{\epsilon}_{i02}-\tilde{\epsilon}_{i\infty 2}}/(\tilde{\epsilon}_{i\infty 2}+2)]\sqrt{\mu_{i2}/m_{ij}(\omega)}\}^2}. \tag{3.4}$$

In order to avoid confusion, it may be necessary to emphasize that the physical parameters in Eq. (3.4) are those of the mixed crystal in the well ($i=1$) or the barrier ($i=2$), where $x_i$ is the concentration, and $\tilde{\epsilon}_{i0l}$ and $\tilde{\epsilon}_{i\infty l}$ $(l=1,2)$ are the optical and static dielectric constants of the end member of the mixed crystal. $\omega_{i1T}$ and $\omega_{i2T}$ are the frequencies of the TO phonons of the end member. $\mu_{i1}$, $\mu_{i2}$, $m_{ij}(\omega)$, and $C_{ij}(\omega)$ are complex functions of the physical parameters of the mixed crystal; readers who are interested in these parameters can refer to the polaron theory of mixed crystals.[21]

## IV. POLARON ENERGY

Within the framework of effective-mass and nondegenerate-band approximations, the total Hamiltonian of the system is expressed as

$$H=\frac{p^2}{2m}+V(z)+\sum_{\beta}\sum_{\mathbf{k}}\hbar\omega_{\beta}(\mathbf{k})a^{\dagger}_{\mathbf{k}\beta}a_{\mathbf{k}\beta}$$

$$+\sum_{\beta}\sum_{\mathbf{k}}[V_{k\beta}L_{k\beta}(z)e^{i\mathbf{k}\cdot\boldsymbol{\rho}}a_{\mathbf{k}\beta}+\text{H.c.}], \tag{4.1}$$

TABLE III. $V_{k\beta}$ in QW's.

| QW | Phonon mode | $j$ | $V_{k\beta}$ |
|---|---|---|---|
| | Confined LO | 1 | $i\sqrt{\frac{2\pi e^2\hbar\omega_{L1}}{Sd\bar{\epsilon}_1}}\frac{1}{\sqrt{k^2+k_m^2}}$ |
| | Half-space LO | 2a,2b | $i\sqrt{\frac{2\pi e^2\hbar\omega_{Lj}}{SD\bar{\epsilon}_{2j}(\omega_{Lj})}}\frac{1}{\sqrt{k^2+k_z^2}}$ |
| *TBT* | Symmetric IO | 1,2,3 | $i\sqrt{\frac{\pi e^2\hbar\omega_{+j}}{Sk}}\left(\bar{\epsilon}_{1+j}(\omega_{+j})\frac{\sinh(2kd)}{\cosh^2(kd)}+\bar{\epsilon}_{2j}(\omega_{+j})\right)^{-1/2}$ |
| | Antisymmetric IO | 1,2,3 | $i\sqrt{\frac{\pi e^2\hbar\omega_{-j}}{Sk}}\left(\bar{\epsilon}_{1-j}(\omega_{-j})\frac{\sinh(2kd)}{\sinh^2(kd)}+\bar{\epsilon}_{2j}(\omega_{-j})\right)^{-1/2}$ |
| | Confined LO | 1*a*,1*b* | $i\sqrt{\frac{2\pi e^2\hbar\omega_{Lj}}{Sd\bar{\epsilon}_{1j}(\omega_{Lj})}}\frac{1}{\sqrt{k^2+k_m^2}}$ |
| | Half-space LO | 2 | $i\sqrt{\frac{2\pi e^2\hbar\omega_{L2}}{SD\bar{\epsilon}_2}}\frac{1}{\sqrt{k^2+k_z^2}}$ |
| *BTB* | Symmetric IO | 1,2,3 | $i\sqrt{\frac{\pi e^2\hbar\omega_{+j}}{Sk}}\left(\bar{\epsilon}_{1j}(\omega_{+j})\frac{\sinh(2kd)}{\cosh^2(kd)}+\bar{\epsilon}_{2+j}(\omega_{+j})\right)^{-1/2}$ |
| | Antisymmetric IO | 1,2,3 | $i\sqrt{\frac{\pi e^2\hbar\omega_{-j}}{Sk}}\left(\bar{\epsilon}_{1j}(\omega_{-j})\frac{\sinh(2kd)}{\sinh^2(kd)}+\bar{\epsilon}_{2-j}(\omega_{-j})\right)^{-1/2}$ |
| | Confined LO | 1*a*,1*b* | $i\sqrt{\frac{2\pi e^2\hbar\omega_{Lj}}{Sd\bar{\epsilon}_{1j}(\omega_{Lj})}}\frac{1}{\sqrt{k^2+k_m^2}}$ |
| | Half-space LO | 2*a*,2*b* | $i\sqrt{\frac{2\pi e^2\hbar\omega_{Lj}}{SD\bar{\epsilon}_{2j}(\omega_{Lj})}}\frac{1}{\sqrt{k^2+k_z^2}}$ |
| *TTT* | Symmetric IO | 1,2,3,4 | $i\sqrt{\frac{\pi e^2\hbar\omega_{+j}}{Sk}}\left(\bar{\epsilon}_{1j}(\omega_{+j})\frac{\sinh(2kd)}{\cosh^2(kd)}+\bar{\epsilon}_{2j}(\omega_{+j})\right)^{-1/2}$ |
| | Antisymmetric IO | 1,2,3,4 | $i\sqrt{\frac{\pi e^2\hbar\omega_{-j}}{Sk}}\left(\bar{\epsilon}_{1j}(\omega_{-j})\frac{\sinh(2kd)}{\sinh^2(kd)}+\bar{\epsilon}_{2j}(\omega_{-j})\right)^{-1/2}$ |

where $V(z)$ is a potential of an electron in the QW. $\mathbf{p}$ and $m$ are the momentum and the effective band mass of the electron, respectively. Since we are now interested in the mixed-crystal effect on the polaron states in the QW's, the simple infinite square potential is used and only the lowest subband state is considered in the present calculation. By using an improved variational method,[11,12] we obtain the expressions of the electron–optical-phonon interaction energies in the three types of the QW's. In the case of *BTB* QW's, if one introduce the lengths in units of the polaron radius $R_p$ $[=(\hbar/2m_e\omega_L)^{1/2}]$, where $\omega_L$ is one of the end-member LO-phonon frequencies of the mixed crystal, and the energy in units of $e^2/2R_p$, then the contributions from slab LO and IO phonon modes can be written as, respectively,

$$E_{\mathrm{LO}}=-\sum_{j=1a,1b}\frac{1}{\bar{\epsilon}_{1j}(\omega_{Lj})}\left\{\frac{3}{4d}\frac{1}{1-\frac{2}{3}(\pi/2d)^2(\omega_L/\omega_{Lj})}\ln\left[\frac{1}{3}+\left(\frac{2d}{\pi}\right)^2\frac{\omega_{Lj}}{\omega_L}\right]+\frac{1}{2d}\sum_{m=2,3,\ldots}\ln\left[1+\left(\frac{2d}{m\pi}\right)^2\frac{\omega_{Lj}}{\omega_L}\right]\right\}, \tag{4.2}$$

$$E_{\mathrm{IO}}=-\sum_j\int dk\,\frac{\omega_{+j}}{\check{\epsilon}_{2+j}\omega_L}\frac{[ee(2kd)+1]^2}{2\cosh^2(kd)\{(\omega_{+j}/\omega_L)[ee(2kd)+1]+2k^2ee(2kd)\}}$$
$$-\sum_j\int dk\,\frac{\omega_{-j}}{\check{\epsilon}_{2-j}\omega_L}\frac{[ee(2kd)-1]^2}{2\sinh^2(kd)\{(\omega_{-j}/\omega_L)[ee(2kd)-1]+2k^2ee(2kd)\}}, \tag{4.3}$$

where $\breve{\epsilon}_{2+j}$ and $\breve{\epsilon}_{2-j}$ are defined by

$$\breve{\epsilon}_{2+j}=\bar{\epsilon}_{1j}(\omega_{+j})\frac{\sinh(2kd)}{\cosh^2(kd)}+\bar{\epsilon}_{2+j}(\omega_{+j}), \tag{4.4}$$

$$\breve{\epsilon}_{2-j}=\bar{\epsilon}_{1j}(\omega_{-j})\frac{\sinh(2kd)}{\sinh^2(kd)}+\bar{\epsilon}_{2-j}(\omega_{-j}), \tag{4.5}$$

and $ee(x)$ is defined by

$$ee(x)=\frac{\pi^2}{x^2+\pi^2}\frac{\sinh(x)}{x}. \tag{4.6}$$

The expressions for the *TBT* and *TTT* QW's can be obtained by the same procedure, which are similar to the above expressions. Here, we do not write them again.

## V. RESULTS AND CONCLUSION

We have derived the expressions of phonon frequencies of all phonon modes, the electron-phonon interaction Hamiltonian, and the expressions of polaron energies in QW's consisting of mixed crystals. As applications, we calculate the concentration dependence of frequencies ($k=0$) and dispersion relations of IO phonons in GaAs/$Ga_xAl_{1-x}As$, $Zn_xCd_{1-x}Se$/ZnSe, and $ZnS_xSe_{1-x}$/ZnS QW's by using the equation listed in Table I. The original data of material parameters are taken from Ref. 22. The first QW is a *TBT* QW in which the barrier is a two-mode mixed crystal. The second is a *BTB* QW, the well is a one-mode mixed crystal. The last is also a *BTB* QW, but the well is a two-mode mixed crystal. The results are plotted in Figs. 1–3. It is shown that there are six IO-phonon modes in the three QW's. The number of IO-phonon modes and the IO-phonon energies obtained here are very different from that obtained with effective-phonon approximation where only four IO modes are in existence. The effect of mixed crystals changes greatly the phonon modes in the QW's consisting of mixed crystal, and will appear in many optical and electronic experiments which relate to the phonon modes and the phonon frequencies. In the past decade, extensive investigations have been carried out on Raman scatting in QW systems. The confined LO-phonon mode and the IO-phonon modes were observed in some QW's.[23,24] We believe that the present theory will be very helpful to the experimenters.

By using the explicit expressions of Eqs. (4.2) and (4.3) one can study the property of the electron–optical-phonon interaction in the QW's. It is noticed that the well-width dependence of the electron–confined-LO-phonon interaction energy in a *BTB* QW is different between the two confined-LO-phonon modes. It is related to the phonon frequency $\omega_{Lj}$ $(j=1a,1b)$ as shown in Eq. (4.2). It is also noticed that the contribution of the confined LO phonons to the interaction energy comes mainly from the phonons with small wave vector $k_m$. The larger the quantum number $m$ the smaller the coupling of the phonon with electrons.

With the expression of the polaron energies, we study numerically the polaronic effects in the QW's. All the phonon modes in the well are taken into consideration. The concentration dependences of the polaron energies in the case of $W=3R_p$ of the QW's are shown in Fig. 4. The contributions due to the confined LO phonons and the IO phonons are also plotted in the figure. Because there are no suitable data for the electron band masses of the mixed crystals, the linear

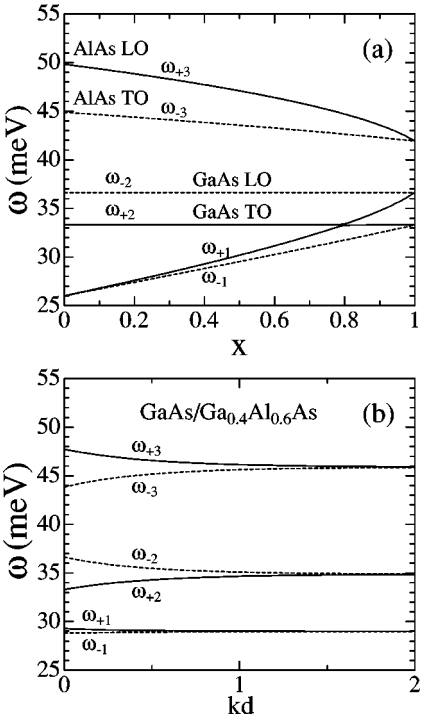


FIG. 1. (a) Concentration dependences of IO-phonon frequencies ($k=0$) in GaAs/$Ga_xAl_{1-x}As$ QW's. (b) Dispersion relations of IO phonons in GaAs/$Ga_{0.4}Al_{0.6}As$ QW's.

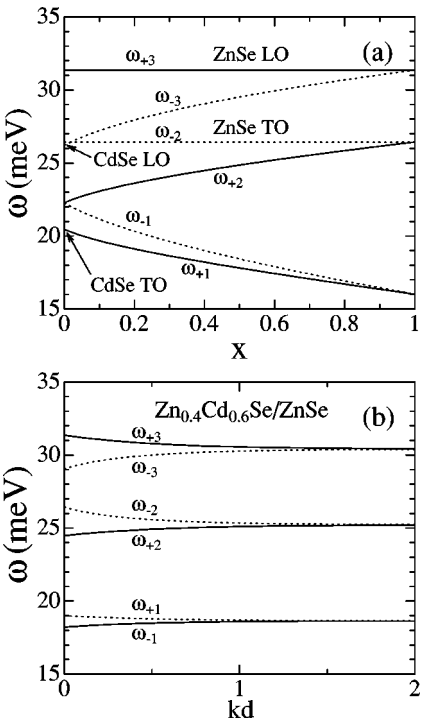


FIG. 2. (a) Concentration dependences of IO-phonon frequencies ($k=0$) in $Zn_xCd_{1-x}Se$/ZnSe QW's. (b) Dispersion relations of IO phonons in $Zn_{0.4}Cd_{0.6}Se$/ZnSe QW's.

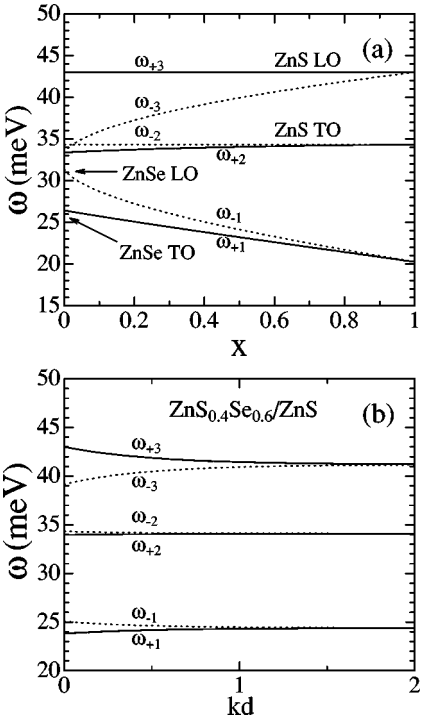


FIG. 3. (a) Concentration dependences of IO-phonon frequencies ($k=0$) in $ZnS_xSe_{1-x}$/ZnS QW's. (b) Dispersion relations of IO phonons in $ZnS_{0.4}Se_{0.6}$/ZnS QW's.

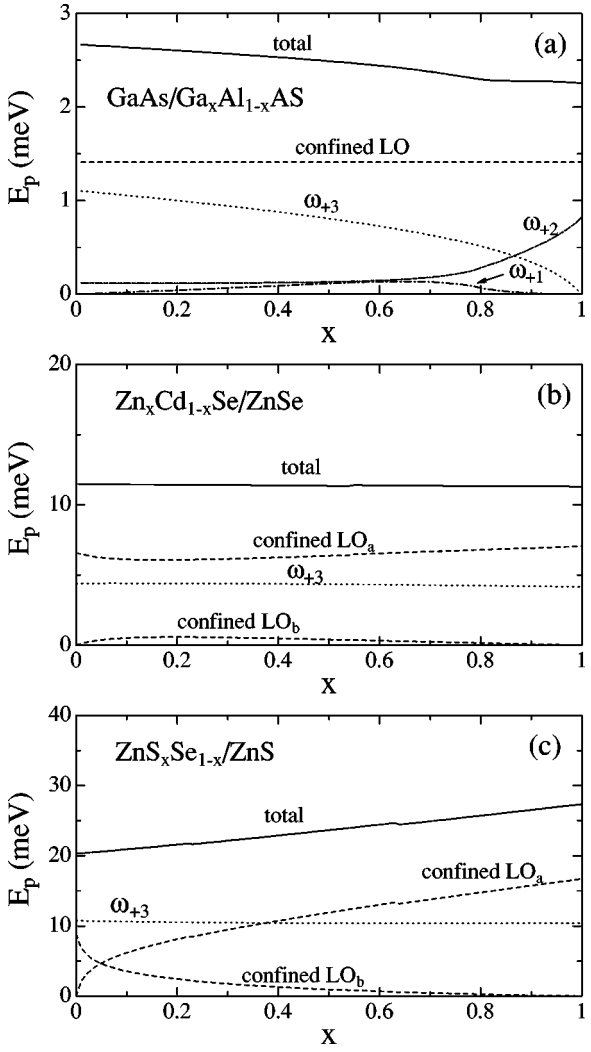


FIG. 4. Electron-phonon interaction energies as functions of the concentration $x$ in the case of $W=3R_p$ in (a) $GaAs/Ga_xAl_{1-x}As$ QW's, (b) $Zn_xCd_{1-x}Se/ZnSe$ QW's, and (c) $ZnS_xSe_{1-x}$/ZnS QW's. The solid line corresponds to the total polaron energy. Dashed lines represent the contributions from the confined LO phonon, and dotted lines are the contributions from the IO phonon.

interpolation method is used to estimate the masses from the two end members of the mixed crystals.

It may be interesting that, as shown in Fig. 4(b), although the well of $Zn_xCd_{1-x}Se$/ZnSe QW's is made of a one-mode mixed crystal and the contribution of the LO phonon mainly comes from the main LO-phonon mode, another weak LO-phonon mode also makes a small contribution to the polaron energy, which is about one-tenth of the contribution of the main LO mode in the composition region of $0.1<x<0.6$ and goes to zero when $x$ goes to 1 or 0. In the case of $ZnS_xSe_{1-x}$/ZnS QW's the well is made of a two-mode mixed crystal, its behavior is very different from the previous one. The importance of the two LO-phonon modes depends on the composition ratio $x$. The contribution of one LO-phonon mode increases with increasing $x$, while on the contrary, the other decreases with increasing $x$.

The polaron energy contributed by the IO phonons is large in the narrow well case and reduces slowly to zero with increasing well width. All the antisymmetric IO-phonon modes almost have no interaction with electrons in the well. In the case of $GaAs/Ga_xAl_{1-x}As$ QW, the contributions to the electron–IO-phonon interaction are mainly from two symmetric IO-phonon modes, $\omega_{+3}$ and $\omega_{+2}$, which correspond to the AlAs-LO-like and GaAs-LO-like modes of the $Ga_xAl_{1-x}As$ alloy. The contribution of the $\omega_{+2}$ mode increases and goes to its largest value as the composition $x$ increases from 0 to 1; at the same time, that of the $\omega_{+3}$ mode decreases from its largest value to zero. In the case of *BTB* QW's, the feature of the IO phonon is very meaningful. The contribution comes almost completely from one symmetric IO-phonon mode ($\omega_{+3}$). The frequency of this IO-phonon mode in the $k\rightarrow 0$ limit is the LO-phonon frequency of the barrier material which is a binary crystal. This fact implies that, as is shown clearly in Figs. 4(b) and 4(c), the effective electron–IO-phonon interaction in *BTB* QW's is independent of the composition ratio $x$ of the well material and will show the feature of the barrier materials. We think this theoretical result is useful for the explanation of some experimental phenomena.

We have also calculated the total polaron energies as a function of the well width and found that the qualitative features are not much different from the results[11] by using the effective-phonon approximation. The reason is simply that the total polaron energy is a sum of the interaction energies of the electron with all of the phonon modes, so that the multimode effects of the phonons are mixed and averaged in this physical quality. This theoretical result seems to be reasonable.

In conclusion, a theory of electron–optical-phonon interactions in QW's consisting of mixed crystals is reported. The number of optical phonon modes, the concentration dependence of phonon frequencies, and the dispersion relations of all IO-phonon modes, and the electron–LO-phonon interac-

tion Hamiltonian of the system are obtained. Expressions of electron-phonon interaction energies in the QW's are given. As applications of the present theory, the concentration dependence and the dispersion relations of the IO-phonon frequencies and the interaction energy of an electron with every optical phonon mode in infinite QW's are calculated numerically. The properties of the polaronic effect in QW's consisting of mixed crystals are discussed. On the basis of the present work, more detailed studies on optical properties, such as Raman scattering, of the QW's consisting of mixed crystals can be done in the future.

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