Optical-phonon modes and Fröhlich potential in one-dimensional quantum-well wires

Bang-fen Zhu
Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100 080, China
and National Laboratory for Superlattices and Microstructures, Institute of Semiconductors,
Chinese Academy of Sciences, P.O. Box 912, Beijing 100 083, China
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By extending our microscopic model on optical-phonon modes in quantum wells to one-dimensional (1D) quantum-well wires (QWW), the optical displacements and associated electrostatic potentials of optical-phonon modes in 1D QWW are calculated. The modes can be clearly divided into confined LO bulklike, TO bulklike modes, and extended interfacelike modes provided the bulk phonon dispersion is ignored. The character of each type of mode is illustrated with special attention to the interfacelike modes, which are hybrids of longitudinal- and transverse-optical waves from the corresponding bulk materials. Based on the numerical results, approximate analytical formulas for bulklike modes are presented. As in 2D wells, both the optical displacements and Fröhlich potentials for the bulklike modes vanish at the interfaces. The finite dispersion of bulk phonons has a more pronounced effect on the 1D phonon modes because interfacelike modes show mixed characteristics of 2D interface and bulklike modes.

The fundamental properties of optical-phonon modes in typical semiconductor superlattice and quantum wells, such as GaAs/AlAs, have become well understood during the past five years.[1-7] Recently, with improvement of sample fabrication technique, one-dimensional quantum-well wires (QWW) attract more and more attention. In contrast to the large number of works on the electronic structure of quasi-one-dimensional (1D) QWW's, to our knowledge, there is no research work on optical-phonon modes in QWW's based on a microscopic model. In this paper, with a specially devised microscopic model,[6,7] which has been justified in dealing with phonon modes in 2D systems, the basic properties of the optical-phonon mode as well as corresponding electrostatic potentials in QWW's are investigated.

As originated by Huang and Rhys[8] and further developed in Ref. 6, a simple cubic lattice of charged oscillators has been used as a model to simulate the relative motion of the oppositely charged particles in a polar lattice. To model optical vibrations in the quantum-well wires constituted of two materials A and B, we shall assume that the A lattice of oscillators differs from the B lattice only in the oscillator's intrinsic frequencies (the difference between squared oscillator frequencies is designated by $\Delta\omega_0^2$). If the z axis is taken to be parallel to the wires, Ma and Na denote, respectively, the rectangular well (A material) widths along the x and y directions, with $M'a$ and $N'a$ representing the corresponding barrier widths, then the period along the x direction is $L_x a$ ($L_x = M + M'$), and the period along the y direction $L_y a$ equals $(N + N')a$, where a is the monolayer width (half lattice constant). Such a rectangular QWW will be denoted as QWW (M,N,M',N'). Thus, among $3L_xL_y$ optical modes, there will be $3MN$ A-like modes and $3(MN' + M'N + M'N')$ B-like modes.

The method of calculation and basic idea are as follows. Similar to the usual effective-mass treatment of electrons and holes in quantum-well wires,[9] the optical vibrational modes can be conveniently imagined as the eigenmodes in the "phonon quantum-well wires," where $\Delta\omega_0^2$ plays the role of the phonon potential barrier height. Owing to QWW periodicity, in working out the A-like optical phonons in QWW's, the eigenmodes can be expanded in terms of LO and TO plane waves of the A lattice, i.e.,

$$|k_{s,p},j\rangle = V^{-1/2}\exp(i\mathbf{k}_{s,p}\cdot\mathbf{R})\hat{\boldsymbol{\epsilon}}(k_{s,p},j) \quad (j=1,2,3,) ,$$

with wave vectors $\mathbf{k}_{s,p}$ related by reciprocal-lattice vectors of the QWW, which can be expressed as

$$\mathbf{k}_{s,p} = \mathbf{k} + (2s\pi/L_x a)\hat{\mathbf{x}} + (2p\pi/L_y a)\hat{\mathbf{y}} ,$$

where s is an integer within $-L_x/2$ and $L_x/2$, and the integer p is between $-L_y/2$ and $L_y/2$. The wave-vector specifying mode in 1D QWW's, $\mathbf{k}=(k_x,k_y,k_z)$, is restricted to the minizone of the QWW lattice. The phonon potential barrier will couple together these A-lattice modes associated with different $\mathbf{k}_{s,p}$, and the following dynamical matrix element can be deduced:

$$\begin{aligned}\langle k_{s',p'},j'|H|k_{s,p},j\rangle = {} & [\omega_A^2(\mathbf{k}_{s,p},j) + \Delta\omega_0^2(1 - MN/L_xL_y)]\delta_{ss'}\delta_{pp'}\delta_{jj'} \\ & + [(1-\delta_{ss'})N'I(s'-s) + (1-\delta_{pp'})M'I(p'-p) \\ & - (1-\delta_{ss'})(1-\delta_{pp'})I(s'-s)I(p'-p)]\hat{\boldsymbol{\epsilon}}^*(\mathbf{k}_{s',p'},j')\cdot\hat{\boldsymbol{\epsilon}}(\mathbf{k}_{s,p},j) ,\end{aligned}$$

where $\omega_A(\mathbf{k}_{s,p},j)$ and $\hat{\epsilon}(\mathbf{k}_{s,p},j)$ are the frequency and normalized displacement of the jth A-lattice mode associated with wave vector $\mathbf{k}_{s,p}$ and

$$I(s-s')=\frac{\Delta\omega_0^2\sin[M(s'-s)\pi/L_x]}{L_xL_y\sin[(s'-s)\pi/L_x]},$$

$$I(p-p')=\frac{\Delta\omega_0^2\sin[N(p'-p)\pi/L_y]}{L_xL_y\sin[(p'-p)\pi/L_y]}.$$

In actual calculations, for a given wave vector, the basis functions of the A lattice are simply assumed to be one LO ($j=1$) and two TO modes ($j=2,3$), with respective parabolic dispersions.

For the sake of convenience in analysis, we first assume that the bulk optical phonons are dispersionless. Later we will take the dispersion effect into account.

Let us first consider the case of modes associated with wave vector perpendicular to the wires, namely, $k_z=0$.

Among the $3MN$ A-like modes, there are MN modes vibrating along the z direction with the TO frequency, which will be denoted as TO2 modes and are characterized by two integers m and n. Their z displacements u_z are well described by a product of two sinusoidal functions of x and y, that is,

$$\sin[m\pi(x/\bar{M}a+0.5)]\sin[n\pi(y/\bar{N}a+0.5)],$$

with $-0.5\bar{M}a<x<0.5\bar{M}a$ and $-0.5\bar{N}a<y<0.5\bar{N}a$. Here $\bar{M}a$ and $\bar{N}a$ represent the QWW effective well widths, with $M+0.5<\bar{M}<M+1$ and $N+0.5<\bar{N}<N+1$. We see that m and n are just the number of half wavelengths contained in the confining layer along the x and y direction, respectively.

The behaviors of the remaining $2MN$ modes vibrating within the xy plane are more complex.

As shown by the calculation, there exist three types of modes. First of all, there are $(M-1)(N-1)$ LO bulklike A modes vibrating at frequency near the bulk LO frequency of the A lattice confined in the well of QWW's (M,N,M',N') for a given wave number vector. That they are $(M-1)(N-1)$ in number rather than MN can be interpreted as follows. Imagine we start with the 2D A material (well) in the superlattice $A_MB_{M'}$, then the B-barrier perturbation in the y direction is introduced to make the QWW (M,N,M',N'). It is known that there exist only $M-1$ branches of A-like LO bulklike modes in the $A_MB_{M'}$ superlattice (the mode with wavelength of $2\bar{M}a$, having the largest net dipole, is strongly coupled with distinct dipoles and is in the nature of the interface mode, thus the bulklike modes will start with $m=2$; cf.

TABLE I. Calculated electrostatic potentials Φ, x displacement u_x, and y displacement u_y, for the first two LO bulklike modes associated with $\mathbf{k}=(0.04\pi/a,0,0)$ in the 1D QWW (5,7,5,5). The figures in front of the parentheses are deduced from the analytical formulas, and the figures inside the parentheses are obtained from the microscopic calculations with zero-dispersion limit (the first) and finite dispersion (the second), respectively. The dispersion parameters are taken from GaAs and AlAs. (a) is for the LO(2,2) mode and (b) is for LO(2,3), where the integers refer to Φ_{mn} in the text.

	y \ x	0	a	$2a$
			(a)	
Φ	0	0.51(0.50,0.50)	0.36(0.36,0.38)	0.09(0.09,0.12)
	a	0.42(0.42,0.42)	0.30(0.31,0.31)	0.07(0.08,0.09)
	$2a$	0.23(0.24,0.23)	0.16(0.17,0.17)	0.04(0.04,0.04)
	$3a$	0.05(0.05,0.04)	0.03(0.04,0.03)	0.01(0.01,0.00)
u_x	0	0.00(0.00,0.00)	0.26(0.25,0.22)	0.22(0.22,0.20)
	a	0.00(0.00,0.00)	0.22(0.21,0.20)	0.18(0.18,0.17)
	$2a$	0.00(0.00,0.00)	0.12(0.12,0.12)	0.10(0.10,0.10)
	$3a$	0.00(0.00,0.00)	0.03(0.03,0.04)	0.02(0.03,0.03)
u_y	0	0.00(0.00,0.00)	0.00(0.00,0.00)	0.00(0.00,0.00)
	a	0.16(0.15,0.16)	0.11(0.11,0.12)	0.03(0.03,0.05)
	$2a$	0.21(0.21,0.22)	0.15(0.15,0.17)	0.04(0.04,0.07)
	$3a$	0.13(0.13,0.13)	0.09(0.09,0.10)	0.02(0.03,0.04)
			(b)	
Φ	0	0.00(0.00,0.00)	0.00(0.00,0.00)	0.00(0.00,0.00)
	a	0.30(0.29,0.28)	0.21(0.21,0.22)	0.05(0.05,0.07)
	$2a$	0.30(0.30,0.31)	0.21(0.22,0.24)	0.05(0.06,0.07)
	$3a$	0.09(0.09,0.11)	0.06(0.06,0.08)	0.02(0.02,0.02)
u_x	0	0.00(0.00,0.00)	0.00(0.00,0.00)	0.00(0.00,0.00)
	a	0.00(0.00,0.00)	0.16(0.15,0.12)	0.13(0.13,0.11)
	$2a$	0.00(0.00,0.00)	0.16(0.15,0.14)	0.13(0.13,0.13)
	$3a$	0.00(0.00,0.00)	0.05(0.05,0.07)	0.04(0.04,0.06)
u_y	0	0.37(0.34,0.36)	0.26(0.25,0.28)	0.06(0.07,0.12)
	a	0.17(0.18,0.20)	0.12(0.13,0.16)	0.03(0.03,0.07)
	$2a$	−0.16(−0.15,−0.11)	−0.11(−0.11,−0.09)	−0.03(−0.03,−0.04)
	$3a$	−0.20(−0.20,−0.17)	−0.14(−0.15,−0.13)	−0.04(−0.04,−0.06)

Ref. 6). Further introduction of the phonon barrier in the y direction leads to a quantization of optical phonons and, consequently, $N-1$ confined modes for each branch of the QW bulklike modes (similarly, the mode with $n=1$ should not be considered as bulklike). It thus turns out that there are $(M-1)(N-1)$ LO bulklike A modes for each QWW wave vector.

In general, the modes polarized within the plane can hardly be expressed by a product of function of x and function of y; however, we have found that, for bulklike modes, especially for the modes associated with longer wavelengths, the mode potentials, which can be considered as the analog of the Fröhlich interaction in 1D quantum systems, are fairly well described by the following analytical expressions (cf. Table I), namely, for even m and n,

$$\Phi_{mn}=R_{mn}^{-1/2}[\cos(m\pi x/\bar{M}a)-(-1)^{m/2}] \times[\cos(n\pi y/\bar{N}a)-(-1)^{n/2}] ;$$

with both odd m and n (3,5,7,...),

$$\Phi_{mn}=R_{mn}^{-1/2}[\sin(\mu_m\pi x/\bar{M}a)+C_m x/\bar{M}a] \times[\sin(\mu_n\pi y/\bar{N}a)+C_n y/\mathrm{Na}] .$$

Here the eigenmode normalization constant R reads

$$R=\int dx\,dy\left[\left[\frac{\partial\Phi}{\partial x}\right]^2+\left[\frac{\partial\Phi}{\partial y}\right]^2+k_j^2\Phi^2\right] ,$$

and the constants μ_n and C_n are the same as given by Ref. 6. Following similar functional relations, one can readily write down the mode potential associated with even m and odd n, or even n and odd m. With the analytical potential functions of vibration modes, the corresponding optical displacements, the derivatives of potentials, are immediately obtained, which are also found to agree with the numerical results. Similar to the 2D bulklike modes, the 1D bulklike mode potentials and the optical displacements both vanish at the interfaces (see Table I).

Besides the LO bulklike modes, there are $(M-1)(N-1)$ bulklike modes with frequencies near the bulk TO frequency, which we designate as TO1-like modes. Their optical displacements are also confined to the A region.

By subtracting the $2(M-1)(N-1)$ bulklike mode from $2MN$ modes, we obtain $2(M+N-1)$ modes, which are found to vibrate at frequencies within the LO-TO gap in the dispersionless limit. This is what should be expected. Since modes with wavelength of $2\bar{M}a$ correspond to two branches of interface modes in the $A_M B_{M'}$ QW, the new period of $L_y a$ in the y direction results in N A modes for each branch of 2D interface modes; on the other hand, periodical variation in the x direction transforms one branch of interface modes in the $A_N B_{N'}$ QW to M A modes containing a $p=0$ component for a given QWW wave vector. Noting that we have twice counted modes associated with $m=1$ and $n=1$, i.e., the mode dominated by the $\mathbf{k}_{0,0}$ component, thus there exist $2(M+N-1)$ A modes affected by the long-range Coulomb interaction sizably; these are designated as interfacelike modes in QWW's. These interfacelike modes are the hybrid of the longitudinal- and transverse-optical waves from the corresponding bulk materials, which are thus in the nature of Coulomb modes,[6] or interface modes. Generally speaking, just as for interface modes in 2D systems, interfacelike mode are accompanied by extended electrostatic potentials and confined optical displacements. Among them, one mode associated with dominant $|\mathbf{k}_{0,0},1\rangle$ component and one with dominant $|\mathbf{k}_{0,0},2\rangle$ component, can be compared to interface modes in 2D systems, which define the band edges for the interfacelike modes if $k_z=0$.

The consideration above provides a guide to numbering the interfacelike modes and indicates that the interfacelike modes, except for two modes dominated by $\mathbf{k}_{0,0}$, have characteristics of both 2D interface and 2D bulklike modes. However, as shown by the numerical results, this does not mean that the displacement or potential function of the interfacelike mode may be characterized as interface mode in one direction and as a bulklike mode in the other direction. In contrast to the bulklike modes in QWW's, interfacelike modes cannot be expressed as a product of two functions of separated variables because of long-range interaction. One noteworthy feature of the interfacelike modes in 1D QWW's is that the frequencies of these modes are split off from the bulk LO and TO bands even in the case of zero k_z, unlike the interface modes with vanishing $\mathbf{k}$ parallel in the 2D QW which merge into the bulklike modes. In the dispersionless limit, the vibration frequencies of these three types of modes are clearly distinguishable (Fig. 1).

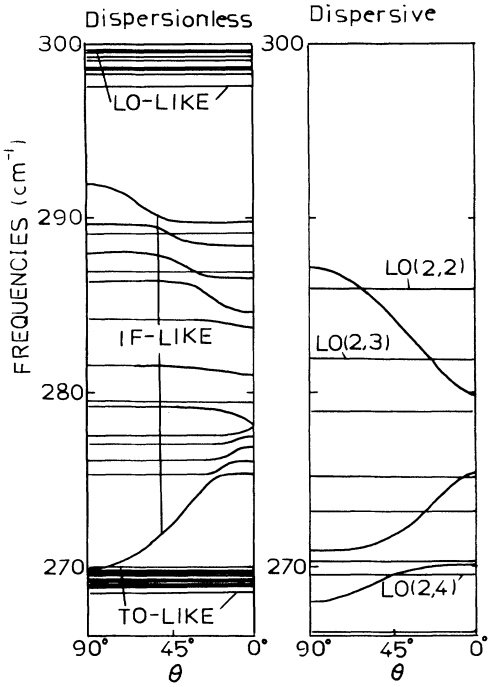

FIG. 1. Long-wavelength frequencies as a function of θ for part of modes in (3,5,3,3) QWW's in the zero phonon dispersion limit (left) and finite phonon dispersion (right), where θ is the angle between the wave vector and the z axis. The notation LO(n,m) refers to Φ_{nm} in the text.

TABLE II. Effect of finite phonon dispersion on mode mixing in the (3,5,3,3) QWW. For wave number as $(0,0,0.04\pi/a)$ and dispersion parameters as Fig. 1, the figures in the first row are the frequencies of the mode in finite dispersion and the percentages are squares of projection of the mode on the modes in the dispersionless limit.

Frequency (cm^{-1})	Percentage of admixture							
286.0	LO(2,2)	75.0	LO(3,2)	10.5				
281.9	LO(2,3)	68.5	LO(3,3)	10.2				
279.8	IF-7	39.5	IF-8	16.7	LO(3,2)	16.2	IF-6	12.1
278.8	IF-2	26.6	IF-5	15.2	LO(2,4)	13.7	IF-1	12.4
275.3	IF-11	49.6	IF-12	34.2				
275.2	IF-9	23.0	LO(3,3)	21.1	IF-13	17.0	IF-6	15.3
273.2	IF-15	33.7	IF-4	23.3				
270.3	IF-15	32.0	IF-4	24.5				
270.1	IF-10	23.1	IF-13	12.5	LO(3,4)	11.8	IF-11	11.4
	IF-14	10.6						
269.5	LO(2,4)	48.6	IF-2	16.9	LO(2,5)	12.3		

For nonvanishing k_z (compared to nonzero k parallel in 2D systems), the TO2(1,1) mode, polarized in the z direction with the longest wavelength, becomes a hybrid of $|\mathbf{k}_{0,0},1\rangle$ and $|\mathbf{k}_{s,p},3\rangle$ $(s,p\neq 0)$ plane waves, forming another interface mode. Thus there are $2(M+N)-1$ interfacelike modes for an oblique QWW wave vector. This interface mode and the upper interface mode polarized in the xy plane dominated by the $\mathbf{k}_{0,0}$ component are $\mathbf{k}$ sensitive, while the others are roughly $\mathbf{k}$ independent. As shown in Fig. 1, when the wave vector changes its direction from perpendicular to the z axis to parallel to the wires, the upper interface mode (at $k_z=0$) decreases its vibration frequency and the TO2(0,0) mode at $k_z=0$ increases the frequency, exhibiting the typical anisotropic dispersion for the interface modes.

In studying phonon modes in 2D systems, we have learned that the finite bulk phonon dispersion plays a special role in determining 2D phonon mode structure. The 2D optical-phonon modes are sharply divided into bulklike modes and interface modes in the limit of zero bulk dispersion; when finite phonon dispersion is taken into account, the interface modes are partially mixed with the bulklike modes with nearby frequencies.[6] In 1D QWW's, however, the dispersion could give rise to even more pronounced change from the clearly separated vibration spectra in the dispersionless limit. Table II lists the square of the projections of several normalized mode vectors calculated in the finite phonon dispersion onto that calculated in the zero-dispersion limit. From the figures, first we can see that, except for such modes as LO(2,2),LO(2,3),... and interface modes associated with dominant $\mathbf{k}_{0,0}$ component (e.g., the 7th, 11th, and 15th interfacelike modes, denoted as IF-7, IF-11, and IF-15, in Table II), other modes are mixed up so heavily that one cannot identify the correspondence between the modes calculated with and without dispersion. Second, the recognizable modes still mix with other modes significantly, though the discrepancies between the analytical expressions and numerical results as given in Table I are generally acceptable. Third, compared with the dispersionless case, not only the bulklike modes, but most interfacelike modes shows remarkably reduced frequencies when dispersion is taken into account. We ascribe such pronounced effects of dispersion on 1D phonon modes to the influences by the relatively large number of interfacelike modes, which have characteristics of both 2D interface and 2D bulklike mode.

So far we have not mentioned the optical-phonon modes in the barrier region. Similar to A modes, there are also two types of B modes: bulklike and interfacelike modes. If $k_z=0$, there exist $2(M+N-1)$ interfacelike modes, $(M'N'+M'N+MN')$ TO2 modes and $[M'N'+1+(M'-1)N+M(N'-1)]$ LO and TO1 bulklike modes. But in this region the bulklike modes exhibit more complicated vibration patterns.

In conclusion, the microscopic model in Refs. 6 and 7 has been applied to investigating optical-phonon modes in 1D quantum wires. The modes are similar to the modes in 2D quantum wells in many aspects, such as dividing modes into bulklike and interfacelike modes, mode mixing induced by finite bulk phonon dispersion, vanishing displacements and potentials at interfaces for bulklike modes, extended potential for the interfacelike modes, etc., but, since the interfacelike modes in 1D systems are different from 2D interface modes, finite dispersion plays a more important role in the 1D phonon spectra.

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