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Polarization eigenvectors of surface-optical phonon modes in a rectangular quantum wire

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The polarization eigenvectors and dispersion relations for confined longitudinal-optical (LO) and surface-optical (SO) phonon modes in a rectangular quantum wire are derived within the continuum approximation. The SO and confined LO modes are compared for a quantum wire with a square cross section in the limit of a vanishing phonon wave vector along the quantum-wire axis. For this case, it is demonstrated that the SO mode becomes dominant over the confined LO modes in interaction with electrons and must be taken into account in calculating the electron–optical-phonon scattering rate.

Epitaxial techniques for the growth of compound-semiconductor structures have advanced to the level where it is possible to fabricate wire-like regions of low-band-gap semiconductor material surrounded completely by regions of higher-band-gap semiconductor material. In particular, such wire-like structures have been realized with rectangular cross sections having small dimensions relative to the thermal de Broglie wavelength.[1] In these structures the electron–optical-phonon scattering rate is affected not only by changes in the electron wave function due to the confining rectangular potential but also by changes in the longitudinal-optical (LO) phonon modes caused by phonon confinement. Fasol *et al.*[2] have recently presented striking experimental evidence of phonon confinement. Size effects on the total scattering rates for polar-optical-phonon scattering of one-dimensional (1D) electron gases in quantum wires and two-dimensional (2D) electron gases in quantum wells have been evaluated previously by Leburton.[3] Recently, Leburton's treatment of 1D electron–LO-phonon scattering was extended by replacing bulk LO-phonon modes with the confined LO-modes of a quantum wire.[4] The scattering rate calculations of Ref. 4 included confined LO-phonon modes of a rectangular wire and neglected electron scattering due to the surface-optical (SO) phonon modes at the quantum-wire boundaries. In this Rapid Communication, the confined LO- and SO-phonon modes are derived for a rectangular quantum wire. In the limit of small (phonon) wave vectors along the quantum-wire axis, it is shown that the contribution of electron–SO-phonon scattering to the ground-state electron–LO-phonon scattering rate becomes significant and cannot be neglected compared to the contribution by the confined LO-phonon modes.

Since the early work of Fuchs and Kliewer,[5,6] the effects of confinement on LO-phonon modes have been studied theoretically by a number of authors for the case of phonon confinement in a quantum well.[7–9] Only recently have confined LO-phonon modes been studied in more complex structures such as quantum wires[4] and strained-layer short-period superlattices.[10,11] In this study, the polarization eigenvectors for the confined LO-phonon and the SO-phonon modes of a quantum wire surrounded by a medium with unity dielectric constant are derived in the continuum approximation.[4,5,7–9] For phonon wavelengths long compared with the lattice constant, continuum models are expected to be valid[5,7,9] and the results of such models agree well with those of microscopic models.[12] The quantum wire is taken to have a dielectric constant ϵ_2, and to be bounded by $\pm L_y/2$ and $\pm L_z/2$ in the y and z directions, respectively. The region surrounding the quantum wire is taken to have a dielectric constant ϵ_1 $(=1)$. The confined LO-phonon modes for such a quantum wire have been given previously.[4]

Since this system is translationally invariant in the x direction, the potential describing the optical-phonon modes may be taken as

$$\Phi(\mathbf{r})=\Phi(y,z)e^{ik_x x}\,, \tag{1}$$

where k_x is the phonon wave vector in the x direction. In the absence of any free charge, the divergence of the displacement vector must vanish and it follows that the potential $\Phi(y,z)$ of the phonon modes must satisfy

$$\epsilon\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-k_x^2\right)\Phi(y,z)=0\,, \tag{2}$$

where $\epsilon=\epsilon_2$ for $-L_y/2<y<+L_y/2$ and $-L_z/2<z<+L_z/2$; outside of this region which defines the quantum wire, $\epsilon=\epsilon_1$. The derivation of Eq. (2) is straightforward upon taking $\mathbf{E}(\mathbf{r})=-\nabla\Phi(\mathbf{r})$, $\mathbf{D}(\mathbf{r})=\epsilon\mathbf{E}(\mathbf{r})=\mathbf{E}(\mathbf{r})+4\pi\mathbf{P}(\mathbf{r})$, and $\Phi(\mathbf{r})$ as given by Eq. (1); a similar treatment has been used previously to arrive at the corresponding result for a quantum well.[8,9] Assuming the y- and z-dependent potentials to be separable and requiring that $\epsilon \neq 0$ for the SO modes, it follows that

$$\frac{1}{\phi_y(y)}\frac{d^2\phi_y(y)}{dy^2}+\frac{1}{\phi_z(z)}\frac{d^2\phi_z(z)}{dz^2}-k_x^2=0\,, \tag{3a}$$

or

$$\alpha^2+\beta^2-k_x^2=0\,, \tag{3b}$$

where $\Phi(y,z)=\phi_y(y)\phi_z(z)$, $\phi_y(y)$ satisfies

$$\frac{d^2\phi_y(y)}{dy^2}=\alpha^2\phi_y(y)\,, \tag{4a}$$

and $\phi_z(z)$ satisfies

$$\frac{d^2\phi_z(z)}{dz^2}=\beta^2\phi_z(z)\,. \tag{4b}$$

Designating $\phi_y(y)$ by $\phi_2(y)$ if $-L_y/2<y<+L_y/2$ and by $\phi_1(y)$ if $|y|>L_y/2$, it follows that $\phi_y(y)$ has a symmetric solution of the form

$$\phi_y^S(y)=\begin{cases}\phi_1^S(y)=Ce^{-\alpha y}, & y>L_y/2\,, \quad (5a)\\ \phi_2^S(y)=Ce^{-\alpha L_y/2}\dfrac{\cosh(\alpha y)}{\cosh(\alpha L_y/2)}, & -L_y/2<y<+L_y/2\,, \quad (5b)\\ \phi_1^S(y)=Ce^{\alpha y}, & y<-L_y/2\,, \quad (5c)\end{cases}$$

and an antisymmetric solution

$$\phi_y^A(y)=\begin{cases}\phi_1^A(y)=Ce^{-\alpha y}, & y>L_y/2\,, \quad (6a)\\ \phi_2^A(y)=Ce^{-\alpha L_y/2}\dfrac{\sinh(\alpha y)}{\sinh(\alpha L_y/2)}, & -L_y/2<y<+L_y/2\,, \quad (6b)\\ \phi_1^A(y)=-Ce^{\alpha y}, & y<-L_y/2\,. \quad (6c)\end{cases}$$

In deriving Eqs. (5) and (6), $\phi_y(y)$ has been taken to be continuous at $|y|=L_y/2$. By further requiring that ϵE_y be continuous at the quantum-wire boundaries, it is necessary that

$$\epsilon_2\tanh(\alpha L_y/2)+\epsilon_1=0 \tag{7a}$$

is the dispersion relation for the symmetric solution and that

$$\epsilon_2\coth(\alpha L_y/2)+\epsilon_1=0 \tag{7b}$$

for the antisymmetric solution. By a similar analysis of Eq. (4b), it is found that the $\phi_z(z)$ satisfies equations of the form of Eqs. (5) and (6) where α, L_y, and y are replaced by β, L_z, and z, respectively. Similarly, the dispersion relations for the symmetric and antisymmetric forms of $\phi_z(z)$ are obtained from Eqs. (7a) and (7b) by replacing α and L_y with β and L_z, respectively. For solutions of $\Phi(y,z)$, where $\phi_y(y)$ and $\phi_z(z)$ are both either symmetric or antisymmetric, it follows that

$$\alpha L_y=\beta L_z\,. \tag{8}$$

Then, Eqs. (8) and (3b) require that

$$\alpha=\frac{k_x}{[1+(L_y/L_z)^2]^{1/2}}\,, \tag{9a}$$

and

$$\beta=\frac{(L_y/L_z)k_x}{[1+(L_y/L_z)^2]^{1/2}}\,. \tag{9b}$$

For solutions of $\Phi(y,z)$ where $\phi_y(y)$ and $\phi_z(z)$ have opposite parities, the dispersion relations for the y and z solution cannot be satisfied simultaneously unless $\cosh[(\alpha L_y-\beta L_z)/2]=0$; accordingly there are no solutions where $\phi_y(y)$ and $\phi_z(z)$ have opposite symmetries. From the stated relationship between **D**, **E**, and **P** in the quantum wire and for $\epsilon_1=1$, the nonvanishing vector is

$$\mathbf{P}_2(\mathbf{r})=\frac{\epsilon_2-1}{4\pi}\mathbf{E}_2(\mathbf{r})=-\frac{\epsilon_2-1}{4\pi}\nabla\Phi_2(\mathbf{r})\,. \tag{10}$$

Taking both $\phi_y(y)$ and $\phi_z(z)$ to be symmetric or antisymmetric and normalizing the nonvanishing polarization modes to unity as in Refs. 5, 7, and 8, the polarization eigenvectors for the symmetric-symmetric mode $\boldsymbol{\pi}^{SS}$ and the antisymmetric-antisymmetric mode $\boldsymbol{\pi}^{AA}$ are

$$\boldsymbol{\pi}^{SS}=\frac{ik_x\cosh(\alpha y)\cosh(\beta z)\hat{x}+\alpha\sinh(\alpha y)\cosh(\beta z)\hat{y}+\beta\cosh(\alpha y)\sinh(\beta z)\hat{z}}{\left[\dfrac{\alpha^2}{2}\left[\dfrac{L_z}{\alpha}\sinh(\alpha L_y)+\dfrac{\sinh(\alpha L_y)\sinh(\beta L_z)}{\alpha\beta}\right]+\dfrac{\beta^2}{2}\left[\dfrac{L_y}{\beta}\sinh(\beta L_z)+\dfrac{\sinh(\alpha L_y)\sinh(\beta L_z)}{\alpha\beta}\right]\right]^{1/2}} \tag{11a}$$

and

$$\boldsymbol{\pi}^{AA}=\frac{ik_x\sinh(\alpha y)\sinh(\beta z)\hat{x}+\alpha\cosh(\alpha y)\sinh(\beta z)\hat{y}+\beta\sinh(\alpha y)\cosh(\beta z)\hat{z}}{\left[\dfrac{\alpha^2}{2}\left[-\dfrac{L_z}{\alpha}\sinh(\alpha L_y)+\dfrac{\sinh(\alpha L_y)\sinh(\beta L_z)}{\alpha\beta}\right]+\dfrac{\beta^2}{2}\left[-\dfrac{L_y}{\beta}\sinh(\beta L_z)+\dfrac{\sinh(\alpha L_y)\sinh(\beta L_z)}{\alpha\beta}\right]\right]^{1/2}}\,, \tag{11b}$$

respectively. Here, $\boldsymbol{\pi}^{SS}$ and $\boldsymbol{\pi}^{AA}$ are the SO-phonon modes for a quantum wire. As discussed above, the dispersion relation for $\boldsymbol{\pi}^{SS}$ is given by Eq. (7a) subject to the condition of Eq. (8); likewise for $\boldsymbol{\pi}^{AA}$ the dispersion relation is Eq. (7b) subject to the condition of Eq. (8). An alternative derivation of the SO-phonon eigenvectors based on an analysis of the normal modes of displacement[9] is currently under way and will be reported shortly. The only major difference in the results of these two approaches is a change in the normalization of the modes.[13]

The polarization eigenvectors for the symmetric-symmetric mode $\boldsymbol{\pi}^{SS}$ and the antisymmetric-antisymmetric mode $\boldsymbol{\pi}^{AA}$ may be compared with the polarization eigenvectors for the confined LO-phonon modes $\boldsymbol{\pi}^{m,n}$, for m and n even and for m and n odd, respectively. The confined LO-phonon modes for a quantum wire discussed in Ref. 4 are obtained in a straightforward manner by computing the normalized eigenvectors corresponding to the phonon potentials $\Phi(y,z)=A_{m,n}\cos(m\pi y/L_y)\times\cos(n\pi z/L_z)$ when both m and n are odd and $\Phi(y,z)=B_{m,n}\sin(m\pi y/L_y)\sin(n\pi z/L_z)$ when both m and n are even. The results are

$$\boldsymbol{\pi}^{m,n}=\frac{ik_x\cos\left(\frac{m\pi}{L_y}y\right)\cos\left(\frac{n\pi}{L_z}z\right)\hat{x}-\left(\frac{m\pi}{L_y}\right)\sin\left(\frac{m\pi}{L_y}y\right)\cos\left(\frac{n\pi}{L_z}z\right)\hat{y}-\left(\frac{n\pi}{L_z}\right)\cos\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)\hat{z}}{\left(\frac{L_yL_z}{4}\right)^{1/2}\left[k_x^2+\left(\frac{m\pi}{L_y}\right)^2+\left(\frac{n\pi}{L_z}\right)^2\right]^{1/2}},\quad\text{with } m,n \text{ odd}, \tag{12a}$$

and

$$\boldsymbol{\pi}^{m,n}=\frac{ik_x\sin\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)\hat{x}+\left(\frac{m\pi}{L_y}\right)\cos\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)\hat{y}+\left(\frac{n\pi}{L_z}\right)\sin\left(\frac{m\pi}{L_y}y\right)\cos\left(\frac{n\pi}{L_z}z\right)\hat{z}}{\left(\frac{L_yL_z}{4}\right)^{1/2}\left[k_x^2+\left(\frac{m\pi}{L_y}\right)^2+\left(\frac{n\pi}{L_z}\right)^2\right]^{1/2}},\quad\text{with } m,n \text{ even}. \tag{12b}$$

The normalization factors in Eqs. (12a) and (12b) result from the normalization conditions specified previously.[5,7,8] They are identical to those obtained from a completely different approach[4] based on deriving the 1D Fröhlich Hamiltonian by imposing appropriate boundary conditions on the 3D Fröhlich Hamiltonian. The y- and z-dependent factors of Eq. (12a) may be obtained from the corresponding factors in $\boldsymbol{\pi}^{SS}$ by replacing α, β, $\cosh(\alpha y)$, $\cosh(\beta z)$, $\sinh(\alpha y)$, and $\sinh(\beta z)$ by $k_y^m=(m\pi/L_y)$, $k_z^n=(n\pi/L_z)$, $\cos(m\pi y/L_y)$, $\cos(n\pi z/L_z)$, $-\sin(m\pi y/L_y)$, and $-\sin(n\pi z/L_z)$, respectively. Likewise, such factors in Eq. (12b) may be obtained from $\boldsymbol{\pi}^{AA}$ by a modified set of substitutions which differs from the above only in that $\sinh(\alpha y)$ and $\sinh(\beta z)$ are replaced by $+\sin(m\pi y/L_y)$ and $+\sin(n\pi z/L_z)$, respectively.

A fundamental distinction between the confined LO-phonon modes of Eqs. (12a) and (12b) and the SO-phonon modes of Eqs. (11a) and (11b) results from the conditions imposed on the SO modes by Eqs. (3b) and (8); namely, the wave vectors in the y and z directions are coupled by k_x as defined by Eqs. (9a) and (9b). In contrast, for the confined LO-phonon modes, $k_y^m=(m\pi/L_y)$ and $k_z^n=(n\pi/L_z)$ are independent of k_x. This important distinction between the SO and LO modes may be illustrated explicitly by considering the special case where $L_y=L_z=L$ and $k_x\to 0$; for this case,

$$\boldsymbol{\pi}^{SS}=\frac{ik_x\hat{x}+\frac{1}{2}k_x^2y\hat{y}+\frac{1}{2}k_x^2z\hat{z}}{k_xL}\xrightarrow[k_x=0]{}\frac{i\hat{x}}{L}, \tag{13a}$$

and

$$\boldsymbol{\pi}^{AA}=\frac{i(\frac{1}{2}k_x^3)yz\hat{x}+\frac{1}{2}k_x^2z\hat{y}+\frac{1}{2}k_x^2y\hat{z}}{(2\sqrt{6})^{-1}k_x^2L^2}\xrightarrow[k_x=0]{}\frac{\sqrt{6}z\hat{y}+\sqrt{6}y\hat{z}}{L^2}. \tag{13b}$$

In calculating the electron-LO-phonon scattering rate in a quantum wire, where the electrons are confined to the ground states in the y and z potentials, the phonon modes with symmetrical phonon potentials are the principal contributors to the scattering overlap integrals. Moreover, in the limit $k_x\to 0$, the symmetric SO-phonon mode yields the polarization eigenvector of Eq. (13a) which has a nonvanishing axis-directed component and vanishing components perpendicular to the quantum-wire interfaces. Accordingly, the interaction potential for this mode scales as $(Lk_x)^{-1}$ and, as a result, the electron-SO-phonon scattering in such a quantum wire will dominate over the electron-LO-phonon scattering rate (due to the confined LO-phonon modes) reported previously by Stroscio.[4] In particular, for $k_x\ll L^{-1}$ it is essential to include the electron-SO-phonon interaction in the calculation of electron-phonon scattering rates in a quantum-wire structure. Specific numerical values for this important effect will be reported in a future publication.[13]

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