Optical-phonon confinement and scattering in wurtzite heterostructures

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We investigate Fröhlich-like electron–optical-phonon interactions in wurtzite structures with single and double heterointerfaces based on the macroscopic dielectric continuum model and the uniaxial model. In addition to confined (for the case of double interfaces), interface, and half-space optical phonon modes as expected from the analogy with zinc-blende structures, propagating modes may exist in wurtzite heterosystems due to anisotropic phonon dispersion. This is especially the case when the dielectric properties of the adjacent heterostructure materials do not differ substantially. The dispersion relations and the interaction Hamiltonians for each of these modes are derived. [S0163-1829(98)09131-0]

I. INTRODUCTION

The optical phonons in wurtzite-based semiconductor structures have begun to receive an increased level of attention due to the progress in applications[1] based on wide-band-gap nitride semiconductors. Since the wurtzite crystals have a different unit-cell structure (i.e., four atoms per unit cell) as well as lower symmetry compared to zinc-blende counterparts, carrier-phonon interactions in this material system differ from those with cubic symmetry. Clearly, there are many more distinct phonon branches (nine optical and three acoustic modes) in wurtzite materials. At the same time, the phonon modes may not be purely longitudinal nor transverse except for the [0001] direction. The understanding of phonon dynamics and their interaction with carriers in wurtzite semiconductors have been primitive.

Very recently, we reported a derivation of the Fröhlich Hamiltonian for *bulk* wurtzite materials[2] based on the macroscopic dielectric continuum model and the uniaxial model of Loudon.[3] The present paper extends this earlier work to study the effects of phonon confinement on electron–optical-phonon interaction Hamiltonians in wurtzite *heterostructures*. The theory of optical-phonon confinement has been treated in detail for zinc-blende structures;[4] however, there do not appear to have been attempts to formulate such a theory for wurtzite structures. The rest of this paper is organized as follows. In Sec. II, basic equations and the derivation of the Fröhlich Hamiltonian for bulk wurtzite materials are summarized for self-sufficiency. In Secs. III and IV, the interaction Hamiltonian is generalized to take into account the role of optical-phonon confinement for wurtzite structures with single and double heterointerfaces, respectively. Concluding remarks follow in Sec. V.

II. FRÖHLICH INTERACTION HAMILTONIAN IN BULK WURTZITE STRUCTURES

Following Loudon,[3] we consider a uniaxial crystal in which only one group of three optical-phonon branches is infrared active; the wurtzite structure is a case in point since at the Γ point, only the $A_1(Z)$ and $E_1(X,Y)$ modes are infrared-active among the nine optical-phonon modes. As discussed in Ref. 3, such a model may be extended to other uniaxial crystals that have larger numbers of polar modes since the method is the same. Within the macroscopic dielectric continuum approach, the field associated with the optical phonon modes in the no-retardation limit satisfies the classical electrostatic equations, i.e.,

$$\mathbf{E}(\mathbf{r}) = -\nabla\Phi(\mathbf{r}), \tag{1}$$

$$\mathbf{D}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) + 4\pi\mathbf{P}(\mathbf{r}) = \epsilon_{\perp}(\omega)E_{\perp}(\mathbf{r})\hat{\rho} + \epsilon_z(\omega)E_z(\mathbf{r})\hat{\mathbf{z}}, \tag{2}$$

$$\nabla\cdot\mathbf{D}(\mathbf{r}) = 0, \tag{3}$$

where $\Phi(\mathbf{r})$ is the electrostatic potential due to the optical-phonon mode, $\mathbf{E}$ is the electric field, $\mathbf{D}$ is the displacement, $\mathbf{P}$ is the polarization field, and $\hat{\mathbf{z}}$ and $\hat{\rho}$ denote the unit vector parallel and perpendicular to the z axis, respectively. When modeling optical phonons for Fröhlich interaction, it is sufficient to consider only the electrostatic boundary conditions;[4] accordingly, in this work we do not take into account the elastic continuum boundary conditions required to model acoustic phonons. In addition, we assume that there is no charge transfer between ions. The expressions and assumptions given above are supported by many studies on the macroscopic dielectric continuum model as surveyed extensively in Ref. 4. Throughout this paper, the z axis is taken along the c direction and the perpendicular direction is denoted as $\perp$. The direction-dependent dielectric functions, $\epsilon_{\perp}(\omega)$ and $\epsilon_z(\omega)$, are given by

$$\epsilon_{\perp}(\omega) = \epsilon_{\perp}^{\infty}\frac{\omega^2-\omega_{\perp L}^2}{\omega^2-\omega_{\perp}^2}, \tag{4}$$

$$\epsilon_z(\omega) = \epsilon_z^{\infty}\frac{\omega^2-\omega_{zL}^2}{\omega^2-\omega_z^2}, \tag{5}$$

where $\omega_{\perp}$ and ω_z are the lattice dispersion frequencies, $\omega_{\perp L}$ and ω_{zL} are the longitudinal-optical (LO) phonon frequen-

cies, and $\epsilon_\perp^\infty$ and ϵ_z^∞ are the high-frequency dielectric constants. Accordingly, the static dielectric constants are $\epsilon_\perp^0 = \epsilon_\perp^\infty \omega_{\perp L}^2/\omega_\perp^2$ and $\epsilon_z^0 = \epsilon_z^\infty \omega_{zL}^2/\omega_z^2$.

The macroscopic equations of motion for uniaxial materials give relations between $\mathbf{E}(\mathbf{r})$, $\mathbf{P}(\mathbf{r})$, and the relative displacement of an ion pair $\mathbf{u}(\mathbf{r})$,[3,5,6]

$$\frac{d^2 u_\perp(\mathbf{r})}{dt^2} = -\omega_\perp^2 u_\perp(\mathbf{r}) + \frac{1}{\sqrt{4\pi\mu n}} \sqrt{\epsilon_\perp^0 - \epsilon_\perp^\infty}\,\omega_\perp E_\perp(\mathbf{r}), \tag{6}$$

$$\frac{d^2 u_z(\mathbf{r})}{dt^2} = -\omega_z^2 u_z(\mathbf{r}) + \frac{1}{\sqrt{4\pi\mu n}} \sqrt{\epsilon_z^0 - \epsilon_z^\infty}\,\omega_z E_z(\mathbf{r}), \tag{7}$$

$$P_\perp(\mathbf{r}) = \sqrt{\frac{\mu n}{4\pi}}\, \sqrt{\epsilon_\perp^0 - \epsilon_\perp^\infty}\,\omega_\perp u_\perp(\mathbf{r}) + \frac{\epsilon_\perp^\infty - 1}{4\pi} E_\perp(\mathbf{r}), \tag{8}$$

$$P_z(\mathbf{r}) = \sqrt{\frac{\mu n}{4\pi}}\, \sqrt{\epsilon_z^0 - \epsilon_z^\infty}\,\omega_z u_z(\mathbf{r}) + \frac{\epsilon_z^\infty - 1}{4\pi} E_z(\mathbf{r}), \tag{9}$$

where μ is the reduced mass and n is the number of unit cells per unit volume. Assuming a harmonic dependence in space and time, we can obtain $\Phi(\mathbf{r})$, $\mathbf{E}(\mathbf{r})$, and $\mathbf{P}(\mathbf{r})$ upon solving Eqs. (1)–(9). Herein, we denote the phonon wave vector as $\mathbf{k}=(\mathbf{q},k_z)$ and define θ as the angle between $\mathbf{k}$ and the z axis. One frequency has a trivial solution: $\omega=\omega_\perp$ and $\mathbf{E}(\mathbf{r})=0$; this is the case for the so-called ordinary phonon. The phonon frequencies for extraordinary phonons are obtained from[3]

$$\epsilon_\perp(\omega)\sin^2\theta + \epsilon_z(\omega)\cos^2\theta = 0. \tag{10}$$

We assume $\epsilon_z^\infty = \epsilon_\perp^\infty$; this is a good assumption since ϵ^∞ is due to electrons. Then,

$$\frac{\omega^2-\omega_{\perp L}^2}{\omega^2-\omega_\perp^2}\sin^2\theta + \frac{\omega^2-\omega_{zL}^2}{\omega^2-\omega_z^2}\cos^2\theta = 0. \tag{11}$$

When we have $|\omega_{\perp L}-\omega_{zL}|, |\omega_\perp-\omega_z| \ll |\omega_{\perp L}-\omega_\perp|, |\omega_{zL}-\omega_z|$, which is the case for the wurtzite-based III–V nitrides, the solutions are

$$\omega^2 = \omega_{zL}^2\cos^2\theta + \omega_{\perp L}^2\sin^2\theta,$$

$$\omega^2 = \omega_z^2\sin^2\theta + \omega_\perp^2\cos^2\theta. \tag{12}$$

These are predominantly longitudinal and transverse modes, respectively. Finally, the electron–optical-phonon Hamiltonian for the bulk uniaxial material is given as[2]

$$H = \sum_q \left[\frac{4\pi e^2\hbar V^{-1}}{(\partial/\partial\omega)(\epsilon_\perp(\omega)\sin^2\theta + \epsilon_z(\omega)\cos^2\theta)}\right]^{1/2} \times \frac{1}{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}(a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger), \tag{13}$$

where V is the crystal volume and $a_{-\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ are the creation and annihilation operators, respectively.

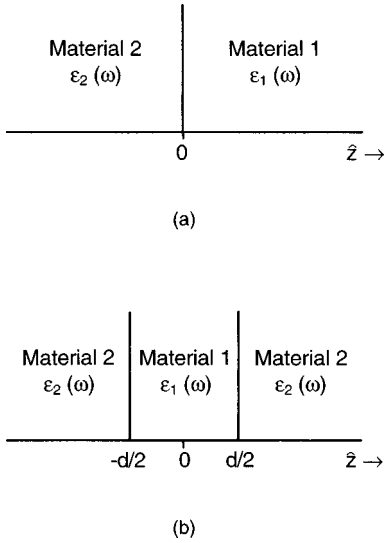

FIG. 1. Schematic drawing of (a) single- and (b) double-heterointerface systems composed of two different wurtzite materials.

III. FRÖHLICH INTERACTION HAMILTONIANS IN WURTZITE STRUCTURES WITH A SINGLE HETEROINTERFACE

Our analysis of optical-phonon confinement effects in wurtzite-based heterostructures begins with the case of structures with a single heterointerface separating two different semi-infinite wurtzite-based semiconductors as shown in Fig. 1(a). One material region, designated by ''1,'' occupies $z>0$ and the other, designated by ''2,'' occupies the region $z<0$. Since there is a translational symmetry perpendicular to the z axis, we have

$$\Phi(\mathbf{r}) = \sum_{\mathbf{q}} \Phi(\mathbf{q},z)e^{i\mathbf{q}\cdot\boldsymbol{\rho}}, \tag{14}$$

where $\mathbf{q}=(k_x,k_y)$ and $\boldsymbol{\rho}=(x,y)$. The boundary conditions at the interface require that $E_\perp$ and D_z be continuous. The normalization condition is given as

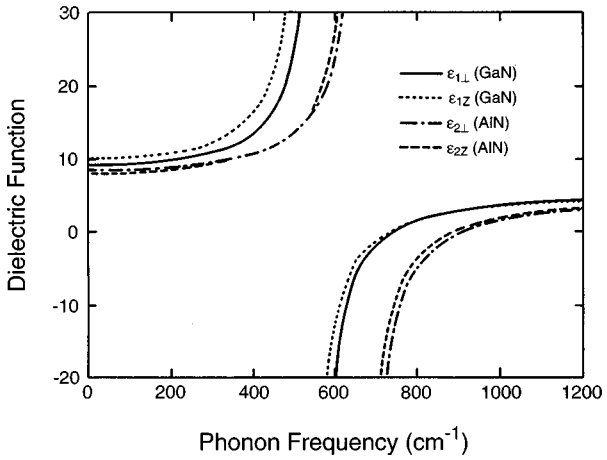

FIG. 2. Frequency dependences of the dielectric constants for materials 1 (GaN) and 2 (AlN). The crystals are of wurtzite symmetry and $\perp$ (z) denotes the direction perpendicular (parallel) to the c axis.

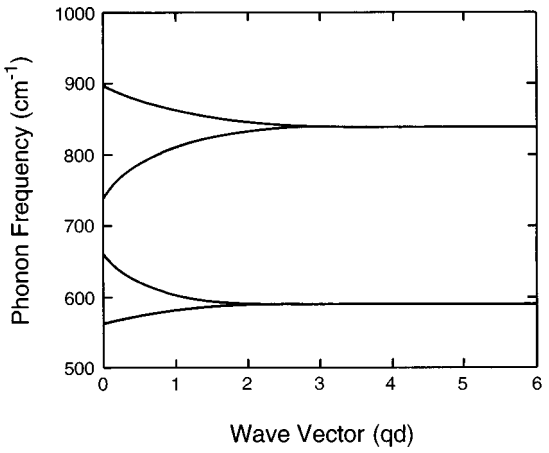

FIG. 3. Dispersion relations for the optical phonon IF modes in an AlN/GaN/AlN double-heterointerface structure.

$$\int \sqrt{\mu n}\mathbf{u}^*(\mathbf{q},z)\cdot\sqrt{\mu n}\mathbf{u}(\mathbf{q},z)dz=\frac{\hbar}{2\omega L^2} \tag{15}$$

and the electron–optical-phonon Hamiltonian can be obtained as

$$H=\sum_{\mathbf{q}} -e\Phi(\mathbf{q},z)e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}}). \tag{16}$$

Here L^2 is the cross-sectional area of the sample.

For the single-heterointerface system under consideration, there may be three distinct classes of optical-phonon modes depending on the ordering of various phonon energy spectra in materials 1 and 2. These modes are designated as interface (IF), half-space (HS), and propagating (PR) modes. The IF modes can exist if solutions can be found for the dispersion relation $\sqrt{\epsilon_{1\perp}\epsilon_{1z}}-\sqrt{\epsilon_{2\perp}\epsilon_{2z}}=0$ with $\epsilon_{1\perp}\epsilon_{1z}>0$, $\epsilon_{2\perp}\epsilon_{2z}>0$, and $\epsilon_{1z}\epsilon_{2z}<0$. The corresponding interaction Hamiltonian can be obtained straightforwardly by following the prescription discussed above and is given as

$$H_{IF}=\sum_{\mathbf{q}}\left[\frac{4\pi e^2\hbar L^{-2}}{|(\partial/\partial\omega)(\sqrt{\epsilon_{1\perp}\epsilon_{1z}}-\sqrt{\epsilon_{2\perp}\epsilon_{2z}})|}\right]^{1/2}\times\frac{1}{\sqrt{q}}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}})\begin{cases}e^{-\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qz}, & z>0\\ e^{\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}qz}, & z<0.\end{cases} \tag{17}$$

This dispersion relation for IF modes is analogous to that of a zinc-blende structure except that, in zinc blendes, the quantities inside the square root are always positive and the frequency range for $\epsilon_1\epsilon_2<0$ exists unless materials 1 and 2 have identical phonon spectra.

The HS mode satisfies the boundary conditions at the heterointerface and behaves as the nominal bulk mode as $z\rightarrow\pm\infty$. Consider the case in which the optical phonon propagates into layer 2 ($z<0$) from layer 1 ($z>0$). The wave vector in layer 1 is denoted by $(\mathbf{q},k_{1z})$, and the angle between $(\mathbf{q},k_{1z})$ and z axis is θ_1. Then, the characteristic phonon frequencies in layer 1 are obtained from Eq. (10) as in bulk material 1. When the solutions of this dispersion relation do not overlap with the optical phonon frequency ranges of material 2 (i.e., between $\omega_{2\perp L}$ and ω_{2zL} or $\omega_{2\perp}$ and ω_{2z}), we have $\epsilon_{2\perp}\epsilon_{2z}>0$ for these modes and the phonon decays exponentially into layer 2. Defining κ_2 as $\kappa_2=\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}q$, the electron–optical-phonon interaction Hamiltonian is

$$H_{HS}=\sum_{\mathbf{q}}\sum_{k_{1z}>0}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{1\perp}\sin^2\theta_1+\epsilon_{1z}\cos^2\theta_1)}\right]^{1/2}\times\frac{1}{\sqrt{q^2+k_{1z}^2}}\frac{2}{\sqrt{\epsilon_{1z}^2k_{1z}^2+\epsilon_{2z}^2\kappa_2^2}}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}})\times\begin{cases}\epsilon_{1z}k_{1z}\cos(k_{1z}z)+\epsilon_{2z}\kappa_2\sin(k_{1z}z), & z>0\\ \epsilon_{1z}k_{1z}e^{\kappa_2 z}, & z<0.\end{cases} \tag{18}$$

The sum should be done only over those k_{1z} that are consistent with $\epsilon_{2z}\epsilon_{2\perp}>0$. The remaining set of HS modes propagating from layer 2 to layer 1 can be considered in the same way.

For special cases where the dielectric properties of the adjacent heterostructure materials do not differ substantially and their dispersion curves overlap, it is possible to establish modes that propagate between adjacent material regions. As an example, we consider the case where the optical phonon in layer 1 propagates also in layer 2. This happens when we have $\epsilon_{2z}\epsilon_{2\perp}<0$ for phonon frequency ω of material 1. Then, the phonon wave vector in layer 2 is $(\mathbf{q},k_{2z})$ with $k_{2z}=\sqrt{-\epsilon_{2\perp}/\epsilon_{2z}}q=\sqrt{\epsilon_{1z}\epsilon_{2\perp}/\epsilon_{1\perp}\epsilon_{2z}}k_{1z}$. There are two possible solutions for these PR modes, quasisymmetric and quasiantisymmetric, whose interaction Hamiltonians are given as

$$H_{PR}^{S}=\sum_{\mathbf{q}}\sum_{k_{1z}>0}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{1\perp}q^2+\epsilon_{1z}k_{1z}^2)+(\partial/\partial\omega)(\epsilon_{2\perp}q^2+\epsilon_{2z}k_{2z}^2)}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}})\begin{cases}2\cos(k_{1z}z), & z>0\\ 2\cos(k_{2z}z), & z<0\end{cases} \tag{19}$$

and

$$H_{PR}^{A}=\sum_{\mathbf{q}}\sum_{k_{1z}>0}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{1\perp}q^2+\epsilon_{1z}k_{1z}^2)\epsilon_{2z}^2k_{2z}^2+(\partial/\partial\omega)(\epsilon_{2\perp}q^2+\epsilon_{2z}k_{2z}^2)\epsilon_{1z}^2k_{1z}^2}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}})\begin{cases}\epsilon_{2z}k_{2z}\sin(k_{1z}z), & z>0\\ \epsilon_{1z}k_{1z}\sin(k_{2z}z), & z<0,\end{cases} \tag{20}$$

respectively. Again, the sum is performed only over those k_{1z} that are consistent with $\epsilon_{2z}\epsilon_{2\perp}<0$. For the isotropic case with $\epsilon_z=\epsilon_\perp$ (for example, the macroscopic dielectric continuum treatment of zinc-blende structures), the PR mode does not exist since $\epsilon_z\epsilon_\perp\geqslant 0$. However, even in zinc-blende structures, such propagating modes were observed experimentally[7] when adjacent regions have small differences in dielectric properties.

Herein, we take GaN for material 1 and AlN for material 2. Material parameters are taken to be $\epsilon^{\infty}=5.29$, $\omega_{\perp L}=743\ \mathrm{cm}^{-1}$, $\omega_{zL}=735\ \mathrm{cm}^{-1}$, $\omega_{\perp}=561\ \mathrm{cm}^{-1}$, $\omega_z=533\ \mathrm{cm}^{-1}$ for GaN.[8] For AlN, we take $\epsilon^{\infty}=4.68$, $\omega_{\perp L}=916\ \mathrm{cm}^{-1}$, $\omega_{zL}=893\ \mathrm{cm}^{-1}$, $\omega_{\perp}=673\ \mathrm{cm}^{-1}$, $\omega_z=660\ \mathrm{cm}^{-1}$.[9] In Fig. 2, the frequency dependences of ϵ_1 (GaN) and ϵ_2 (AlN) are depicted along with the longitudinal and transverse frequencies of interest. As can be seen from this figure, there is no frequency range that satisfies $\epsilon_{1\perp}\epsilon_{1z}<0$ and $\epsilon_{2\perp}\epsilon_{2z}<0$ simultaneously (i.e., no overlap in characteristic frequencies). Hence only IF and HS modes exist in GaN/AlN heterostructures with a single interface.

IV. FRÖHLICH INTERACTION HAMILTONIANS IN WURTZITE STRUCTURES WITH TWO HETEROINTERFACES

In this section, the optical phonon modes and the Fröhlich interaction Hamiltonians are derived for wurtzite structures having two heterointerfaces. Figure 1(b) depicts the structure considered in this section. For such double-heterointerface systems, there may be four distinct classes of optical-phonon modes. Similar to Sec. III, these modes are designated as IF, confined, HS, and PR optical modes. As for the zinc-blende case, there are two types (symmetric and antisymmetric) of IF phonons. For the symmetric mode, the interaction Hamiltonian is given as

$$H_{IF}^{S}=\sum_{\mathbf{q}}\left[\frac{4\pi e^2\hbar L^{-2}}{\left|(\partial/\partial\omega)\left(\sqrt{\epsilon_{1\perp}\epsilon_{1z}}\tanh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right)-\sqrt{\epsilon_{2\perp}\epsilon_{2z}}\right)\right|}\right]^{1/2}\frac{1}{\sqrt{2q}}\,e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\left(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger}\right)$$
$$\times\begin{cases}\cosh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qz\right)/\cosh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right), & |z|<d/2\\ e^{-\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}q(|z|-d/2)}, & |z|>d/2.\end{cases}\tag{21}$$

The frequency ω is determined from $\sqrt{\epsilon_{1\perp}\epsilon_{1z}}\tanh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right)-\sqrt{\epsilon_{2\perp}\epsilon_{2z}}=0$ with $\epsilon_{1z}\epsilon_{2z}<0$ ($\epsilon_{1\perp}\epsilon_{1z}>0$ and $\epsilon_{2\perp}\epsilon_{2z}>0$). For the antisymmetric mode, it is

$$H_{IF}^{A}=\sum_{\mathbf{q}}\left[\frac{4\pi e^2\hbar L^{-2}}{\left|(\partial/\partial\omega)\left(\sqrt{\epsilon_{1\perp}\epsilon_{1z}}\coth\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right)-\sqrt{\epsilon_{2\perp}\epsilon_{2z}}\right)\right|}\right]^{1/2}\frac{1}{\sqrt{2q}}\,e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\left(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger}\right)$$
$$\times\begin{cases}\sinh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qz\right)/\sinh\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right), & |z|<d/2\\ \mathrm{sgn}(z)e^{-\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}q(|z|-d/2)}, & |z|>d/2,\end{cases}\tag{22}$$

and the associated dispersion relationship is $\sqrt{\epsilon_{1\perp}\epsilon_{1z}}\coth\left(\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}qd/2\right)-\sqrt{\epsilon_{2\perp}\epsilon_{2z}}=0$ with $\epsilon_{1z}\epsilon_{2z}<0$. The dispersion relations for the IF modes of a wurtzite AlN/GaN/AlN quantum well with thickness d are depicted in Fig. 3.

The confined modes in double-heterointerface structures may be classified into two groups: one for symmetric confined modes and one for antisymmetric confined modes. For the symmetric modes, the carrier–optical-phonon interaction Hamiltonian is given by

$$H_{C}^{S}=\sum_{\mathbf{q}}\sum_{m}\left[\frac{4\pi e^2\hbar L^{-2}}{(\partial/\partial\omega)(\epsilon_{1\perp}q^2+\epsilon_{1z}k_{1m}^2)d/2-2q(\partial/\partial\omega)f_s(\omega)\cos(k_{1m}d/2)}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\left(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger}\right)$$
$$\times\begin{cases}\cos(k_{1m}z), & |z|<d/2\\ \cos(k_{1m}d/2)e^{-\kappa_2(|z|-d/2)}, & |z|>d/2,\end{cases}\tag{23}$$

where $f_s(\omega)=\mathrm{sgn}(\epsilon_{1z})\sqrt{-\epsilon_{1\perp}(\omega)\epsilon_{1z}(\omega)}\sin(k_{1m}d/2)-\mathrm{sgn}(\epsilon_{2z})\sqrt{\epsilon_{2\perp}(\omega)\epsilon_{2z}(\omega)}\cos(k_{1m}d/2)$. k_{1m} is determined from $\epsilon_{1z}k_{1m}\sin(k_{1m}d/2)-\epsilon_{2z}\kappa_2\cos(k_{1m}d/2)=0$ with $2m\pi/d<k_{1m}<2(m+1)\pi/d$ and κ_2 is given by $\kappa_2=\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}q$. As for the case of zinc-blende confined phonons, the index, m in Eq. (23) runs over the series of confined modes. For the antisymmetric mode,

$$H_{C}^{A}=\sum_{\mathbf{q}}\sum_{m}\left[\frac{4\pi e^2\hbar L^{-2}}{(\partial/\partial\omega)(\epsilon_{1\perp}q^2+\epsilon_{1z}k_{1m}^2)d/2-2q(\partial/\partial\omega)f_a(\omega)\sin(k_{1m}d/2)}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\left(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger}\right)$$
$$\times\begin{cases}\sin(k_{1m}z), & |z|<d/2\\ \mathrm{sgn}(z)\sin(k_{1m}d/2)e^{-\kappa_2(|z|-d/2)}, & |z|>d/2,\end{cases}\tag{24}$$

where $f_a(\omega)=\mathrm{sgn}(\epsilon_{1z})\sqrt{-\epsilon_{1\perp}(\omega)\epsilon_{1z}(\omega)}\cos(k_{1m}d/2)+\mathrm{sgn}(\epsilon_{2z})\sqrt{\epsilon_{2\perp}(\omega)\epsilon_{2z}(\omega)}\sin(k_{1m}d/2)$. k_{1m} is determined from $\epsilon_{1z}k_{1m}\cos(k_{1m}d/2)+\epsilon_{2z}\kappa_2\sin(k_{1m}d/2)=0$ with $(2m-1)\pi/d<k_{1m}<(2m+1)\pi/d$ ($m=1,2,3,\ldots$) and κ_2 is $\kappa_2=\sqrt{\epsilon_{2\perp}/\epsilon_{2z}}q$.

For the case of HS modes, the application of the boundary condition of continuous $E_{\perp}$ and D_z at each interface, as well as the condition that the modes behave as bulk modes as $z\rightarrow\pm\infty$, lead to an HS-mode interaction Hamiltonian similar to those in zinc-blende structures. We denote the angle between $(\mathbf{q},k_{2z})$ and the z axis as θ_2. Then, as in Sec. III, the phonon

frequencies for two outside layers are obtained from Eq. (10) with a proper application of parameters for material 2. Taking $\epsilon_{1\perp}\epsilon_{1z}>0$ (otherwise, the mode belongs to the PR phonons), we define κ_1 as $\kappa_1=\sqrt{\epsilon_{1\perp}/\epsilon_{1z}}q$ and the electron–optical-phonon interaction Hamiltonian for the symmetric case is

$$H_{HS}^{S}=\sum_{\mathbf{q}}\sum_{k_{2z}}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{2\perp}\sin^2\theta_2+\epsilon_{2z}\cos^2\theta_2)}\right]^{1/2}\frac{e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger})}{\sqrt{q^2+k_{2z}^2}}\sqrt{2}/[\epsilon_{1z}^2\kappa_1^2\sinh^2(\kappa_1 d/2)+\epsilon_{2z}^2k_{2z}^2\cosh^2(\kappa_1 d/2)]^{1/2}$$
$$\times\begin{cases}\epsilon_{1z}\kappa_1\sinh\left(\kappa_1\dfrac{d}{2}\right)\sin\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]+\epsilon_{2z}k_{2z}\cosh\left(\kappa_1\dfrac{d}{2}\right)\cos\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right], & |z|>d/2\\ \epsilon_{2z}k_{2z}\cosh(\kappa_1 z), & |z|<d/2.\end{cases}\tag{25}$$

The sum is over k_{2z} (not over k_{1z}) and should be done only for those k_{2z} which satisfy $\epsilon_{1\perp}\epsilon_{1z}>0$. For the antisymmetric case,

$$H_{HS}^{A}=\sum_{\mathbf{q}}\sum_{k_{2z}}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{2\perp}\sin^2\theta_2+\epsilon_{2z}\cos^2\theta_2)}\right]^{1/2}\frac{e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger})}{\sqrt{q^2+k_{2z}^2}}\sqrt{2}/[\epsilon_{1z}^2\kappa_1^2\cosh^2(\kappa_1 d/2)+\epsilon_{2z}^2k_{2z}^2\sinh^2(\kappa_1 d/2)]^{1/2}$$
$$\times\begin{cases}\mathrm{sgn}(z)\left\{\epsilon_{1z}\kappa_1\cosh\left(\kappa_1\dfrac{d}{2}\right)\sin\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]+\epsilon_{2z}k_{2z}\sinh\left(\kappa_1\dfrac{d}{2}\right)\cos\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]\right\}, & |z|>d/2\\ \epsilon_{2z}k_{2z}\sinh(\kappa_1 z), & |z|<d/2.\end{cases}\tag{26}$$

Finally, based on the procedures of Sec. III, we find that the PR modes have the following interaction Hamiltonians for symmetric and antisymmetric cases, respectively:

$$H_{PR}^{S}=\sum_{\mathbf{q}}\sum_{k_{2z}}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{2\perp}q^2+\epsilon_{2z}k_{2z}^2)}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger})\sqrt{2}/[\epsilon_{1z}^2k_{1z}^2\sin^2(k_{1z}d/2)+\epsilon_{2z}^2k_{2z}^2\cos^2(k_{1z}d/2)]^{1/2}$$
$$\times\begin{cases}\epsilon_{2z}k_{2z}\cos\left(k_{1z}\dfrac{d}{2}\right)\cos\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]-\epsilon_{1z}k_{1z}\sin\left(k_{1z}\dfrac{d}{2}\right)\sin\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right], & |z|>d/2\\ \epsilon_{2z}k_{2z}\cos(k_{1z}z), & |z|<d/2,\end{cases}\tag{27}$$

$$H_{PR}^{A}=\sum_{\mathbf{q}}\sum_{k_{2z}}\left[\frac{4\pi e^2\hbar L^{-3}}{(\partial/\partial\omega)(\epsilon_{2\perp}q^2+\epsilon_{2z}k_{2z}^2)}\right]^{1/2}e^{i\mathbf{q}\cdot\boldsymbol{\rho}}(a_{\mathbf{q}}+a_{-\mathbf{q}}^{\dagger})\sqrt{2}/[\epsilon_{1z}^2k_{1z}^2\cos^2(k_{1z}d/2)+\epsilon_{2z}^2k_{2z}^2\sin^2(k_{1z}d/2)]^{1/2}$$
$$\times\begin{cases}\mathrm{sgn}(z)\left\{\epsilon_{2z}k_{2z}\sin\left(k_{1z}\dfrac{d}{2}\right)\cos\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]+\epsilon_{1z}k_{1z}\cos\left(k_{1z}\dfrac{d}{2}\right)\sin\left[k_{2z}\left(|z|-\dfrac{d}{2}\right)\right]\right\}, & |z|>d/2\\ \epsilon_{2z}k_{2z}\sin(k_{1z}z), & |z|<d/2.\end{cases}\tag{28}$$

Once q and k_{2z} are given, ω is determined. Here, $\Sigma_{k_{2z}}$ denotes a sum over those k_{2z} that satisfy $\epsilon_{1\perp}\epsilon_{1z}<0$. As discussed in Sec. III, the PR modes do not exist in the AlN/GaN system.

V. CONCLUSION

The Hamiltonians for the Fröhlich interactions presented in this paper are essential for describing a broad class of carrier–optical-phonon interactions in single- and double-heterointerface wurtzite-based structures when it is necessary to model such interactions in the vicinity of heterostructure interfaces. More specifically, for wurtzite structures with relatively little anisotropy between the parallel and perpendicular dielectric properties (with respect to the c axis), it is clear that phonon confinement effects are important for distances within about 10 nm of a heterostructure interface.[4] For the case of anisotropic dielectric properties, it is expected that confinement effects will occur on roughly the same dimensional scale but it is crucial that the exact theory developed in the present paper be taken into account including the possibility of PR modes. Thus, our results will be valuable for understanding the electronic and optical properties of wurtzite-based heterostructures that advanced growth technologies[8,10,11] are currently making available for both basic and applied studies.

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