Dispersion of polar optical phonons in wurtzite quantum wells

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Dispersion relations for polar optical phonon modes in wurtzite quantum wells (QW's) are obtained in the framework of the dielectric continuum model. It is found that anisotropy of the dielectric medium causes a number of qualitative peculiarities in the phonon spectra. Among these are the absence of the proper confinement for the oscillatory waves located in the QW, inversion of the order of symmetric and antisymmetric quasiconfined optical modes, formation of the finite energy intervals where such confined modes—which are found to be dispersive—can exist, penetration of the half-space phonons into the QW, etc. Some additional peculiarities, such as appearance of propagating modes, strong dispersion of long-wavelength half-space modes, and reduction of the number of interface modes, arise as a result of overlapping characteristic phonon frequencies of the surrounding material and the material of QW. Predicted phonon behavior leads to the conclusion that dependence of dielectric properties of ternary-binary low-dimensional wurtzite heterostructures on composition can serve as a powerful tool for the purposes of phonon spectrum engineering. In order to illustrate these results, the optical phonon spectra are calculated for an $Al_{0.15}Ga_{0.85}N/GaN/Al_{0.15}Ga_{0.85}N$ QW, an AlN/GaN/AlN QW, and for a GaN dielectric slab. [S0163-1829(99)05907-X]

I. INTRODUCTION

High optical efficiency and strong atomic bonding, which are characteristics of GaN, make this material attractive as a basis for the creation of reliable high-power devices able to work in extreme environmental conditions. Recent progress achieved in growth technology, such as the growth of high-quality GaN on sapphire substrates using AlN buffers,[1] as well as the creation of a blue laser diode based on GaN (Ref. 2) have stimulated a new wave of interest in the nitrides. In this material system with hexagonal symmetry, optical phonons play a dominant role in energy dissipation processes as a result of the difference in anion and cation masses. As is known for the case of zinc-blende materials, the presence of heterointerfaces dramatically changes the spectrum of the optical vibrations and leads to the appearance of the confined, interface, and half-space modes.[3] Due to the dielectric anisotropy caused by the lower symmetry of the wurtzites, one can expect that the spectrum of optical phonons in wurtzite-based low-dimensional structures will manifest some additional peculiarities. Since knowledge of the phonon spectra in nanostructures is necessary to understand phonon-electron interactions and other phonon-related processes, we investigate the characteristics of polar optical vibrations in wurtzite heterostructures in the present paper. Particularly, we specify these peculiarities for a case when the optical axis is perpendicular to the heterointerface using a free-standing GaN quantum well/slab (FSQW) and $Al_xGa_{1-x}N/GaN/Al_xGa_{1-x}N$ heterostructures as an illustration. Our treatment is based on the approach developed by Loudon[4] for uniaxial crystals and the macroscopic dielectric continuum model.[5]

The paper is organized as follows. General remarks regarding details of the approach are given in Sec. II. Section III is devoted to the derivation of the optical-phonon modes in wurtzite dielectric slabs and QW's. Results are discussed in Sec. IV and summarized in Sec. V.

II. ASSUMPTIONS

We take the z axis along the direction of the crystallographic c axis, which is assumed to be perpendicular to the heterointerfaces. The width of the well is d and the z coordinates of the interfaces are $\mp d/2$. The frequency-dependent dielectric functions are

$$\epsilon_z(\omega)=\epsilon_z^{\infty}\frac{\omega^2-\omega_{Lz}^2}{\omega^2-\omega_z^2},\quad \epsilon_t(\omega)=\epsilon_t^{\infty}\frac{\omega^2-\omega_{Lt}^2}{\omega^2-\omega_t^2}, \tag{1}$$

where ω_{Lz}, ω_z, ω_{Lt}, and ω_t are the characteristic frequencies of $A_1(LO)$, $A_1(TO)$, $E_1(LO)$, and $E_1(TO)$ modes, respectively. The subscript t denotes the direction perpendicular to the z axis. We assume that, for a given material, the relation $\epsilon_z^{\infty}=\epsilon_t^{\infty}$ is satisfied with good accuracy.

The phonon potential is taken to have the form $\Phi(r)=\Phi(z)e^{i\vec{q}\cdot\vec{\rho}}$, where $\vec{q}$ and $\vec{\rho}$ are the two-dimensional phonon wave vector and the radius vector in plane (x,y), respectively. We will consider the case of free oscillations:

$$\nabla\cdot\vec{D}=\left[\epsilon_z(\omega)\frac{\partial^2}{\partial z^2}-\epsilon_t(\omega)q^2\right]\Phi(r)=0, \tag{2}$$

with standard boundary conditions (BC's) for the z component of the displacement vector $\vec{D}$ and the tangential component of the electric field $\vec{E}$ at the interfaces:

$$-\epsilon_{2z}(\omega)\left.\frac{\partial\Phi_2(z)}{\partial z}\right|_{z=\mp d/2}=-\epsilon_{1z}(\omega)\left.\frac{\partial\Phi_1(z)}{\partial z}\right|_{z=\mp d/2},$$

$$\Phi_2(z)|_{z=\mp d/2}=\Phi_1(z)|_{z=\mp d/2}. \tag{3}$$

Throughout this paper, we will use index 1 for the material of the QW and index 2 for the surrounding material.

In a crystal with wurtzite structure, there are two types of phonon waves:[4] (a) ordinary waves, where for any angle θ between the phonon wave vector $\vec{\kappa}=(\vec{\kappa}_z,\vec{q})$ and the c axis, both the electric field $\vec{E}$ and the polarization $\vec{P}$ are perpendicular to the c axis and $\vec{\kappa}$ simultaneously, and (b) extraordinary waves, for which the orientation of $\vec{E}$ and $\vec{P}$ with respect to $\vec{\kappa}$ and the c axis is more complicated. Assuming $\vec{E}$ and $\vec{P}\ \propto e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}$ and neglecting retardation effects, the ordinary phonons become the transverse lattice vibrations relative to the c axis and have $\vec{E}=0$. In light of this fact, the present article will consider only extraordinary phonons for which $\vec{E}\|-\vec{\kappa}$ for the given assumptions.

The dispersion relation for the extraordinary bulk phonons is

$$\epsilon_t(\omega)\sin^2\theta+\epsilon_z(\omega)\cos^2\theta=0. \tag{4}$$

For the chosen geometry, Eq. (4) reduces to

$$\epsilon_t(\omega)q^2+\epsilon_z(\omega)\kappa_z^2=0. \tag{5}$$

Herein, we assume that both q and ω are real and positive. This implies that the z component of the phonon wave vector, κ_z, can be either purely real or purely imaginary depending on the sign of $\epsilon_z\epsilon_t$ in each medium. Thus, we have

$$\epsilon_z(\omega)\epsilon_t(\omega)<0,\quad \mathrm{Im}[\kappa_z]=0\ \text{ for oscillating waves,} \tag{6a}$$

and

$$\epsilon_z(\omega)\epsilon_t(\omega)>0,\quad \mathrm{Re}[\kappa_z]=0\ \text{ for decaying waves.} \tag{6b}$$

At each given ω, the conditions of Eqs. (6a) and (6b) determine the character of the modes in each region (confined, interface, etc.).

III. OPTICAL PHONON MODES IN WURTZITE QUANTUM WELLS

A. Confined modes

In an optically isotropic QW, proper confinement of the phonon modes is possible since the BC's for the oscillatory waves in the QW require zero potential both at the interface and throughout medium 2. As a result, the confined (C) modes have no dispersion and are characterized by discrete values of the phonon wavenumber q. Breaking of the spherical dielectric symmetry, however, forbids the existence of the dispersionless confined waves since for this case, the condition $\epsilon_t(\omega)=\epsilon_z(\omega)=\epsilon(\omega)=0$ cannot be satisfied. Moreover, since the anisotropy of frequency-dependent dielectric function implies $\epsilon_{1,2z}(\omega)\neq 0|_{q\neq 0}$ and $\epsilon_{1z}(\omega)\neq\epsilon_{2z}(\omega)$, the BC's of Eq. (3) for a mode spatially localized in the z direction inevitably lead to finite potential at the interface and, consequently, to the penetration of a phonon with frequency ω into medium 2. For this account, we define C modes in a wurtzite-based QW as modes that satisfy the conditions of Eqs. (6a) and (6b) in media 1 and 2, respectively. Thus, confinement for the phonon modes in a wurtzite QW ($c\|z$) means that the modes are localized *around* rather then confined inside an embedded QW and are characterized by finite dispersion that leads to the formation of a band of allowed frequencies.

For the confined modes, by applying the additional BC

$$\Phi_2(z)|_{z\to\mp\infty}=0 \tag{7}$$

one can obtain the following set of equations:

$$\begin{aligned}
&Q_m\{[\mu\xi_2\cos(\alpha Q_m)-\xi_1\sin(\alpha Q_m)]A\\
&\quad+[-\mu\xi_2\sin(\alpha Q_m)-\xi_1\cos(\alpha Q_m)]B\}=0,\\
&Q_m\{[-\mu\xi_2\cos(\alpha Q_m)+\xi_1\sin(\alpha Q_m)]A\\
&\quad+[-\mu\xi_2\sin(\alpha Q_m)-\xi_1\cos(\alpha Q_m)]B\}=0,
\end{aligned} \tag{8}$$

where $\mu=\mathrm{sign}[\epsilon_{1z}(\omega)\epsilon_{2z}(\omega)]$, $\xi_1=\sqrt{|\epsilon_{1z}(\omega)\epsilon_{1t}(\omega)|}$, $\xi_2=\sqrt{|\epsilon_{2z}(\omega)\epsilon_{2t}(\omega)|}$, $\alpha=\frac{1}{2}\sqrt{|\epsilon_{1,t}(\omega)/\epsilon_{1,z}(\omega)|}$, $Q_m=q_md$, and m is the quantum number for even and odd confined modes. To find the full system of nontrivial solutions for $Q_m=Q_m(\omega)$, we transform the set of equations denoted by Eq. (8) into

$$\begin{aligned}
&\sin[\alpha Q_m+\mu\arctan(\xi_1/\xi_2)]=0\\
&\quad\text{for antisymmetric modes } (A=0),\\
&\sin[\alpha Q_m-\mu\arctan(\xi_2/\xi_1)]=0\\
&\quad\text{for symmetric modes } (B=0).
\end{aligned} \tag{9}$$

Finally, the dispersion relation becomes

$$\begin{aligned}
Q_m^a&=[m\pi-\mu\arctan(\xi_1/\xi_2)]/\alpha\\
&\quad\text{for antisymmetric modes}\\
&\quad(m=1,2,3\ldots\ \text{and}\ 0\ \text{if}\ \mu=-1),\\
Q_m^s&=[m\pi+\mu\arctan(\xi_2/\xi_1)]/\alpha\\
&\quad\text{for symmetric modes}\\
&\quad(m=1,2,3\ldots\ \text{and}\ 0\ \text{if}\ \mu=1).
\end{aligned} \tag{10}$$

The dispersion relation for a FSQW can be obtained by setting $\xi_2\equiv 1$ in Eq. (10). It is straightforward to show that for the isotropic case, the dispersion relation of Eq. (10) transforms to the well-known discrete values of q_m. Indeed, taking into account that for an isotropic medium $\xi_1=0$ and $\alpha=1/2$, we have $q'_m=m'\pi/d\neq q(\omega)$ with $m'=1,3,5\ldots$ for symmetric and $m'=2,4,6\ldots$ for antisymmetric modes, respectively.

B. Interface modes

The interface (IF) modes are the evanescent modes with maximum amplitude at the interfaces. For these modes, the

requirement $\epsilon_{1z}\epsilon_{2z}<0$ must be satisfied along with the condition of Eq. (6b) in both media. Applying appropriate BC's for the interface modes, the dispersion relation can be found as

$$Q^a=\frac{1}{2}\ln\left[\frac{\xi_1+\xi_2}{\xi_2-\xi_1}\right]/\alpha \quad \text{for antisymmetric modes},$$
$$Q^s=\frac{1}{2}\ln\left[\frac{\xi_1+\xi_2}{\xi_1-\xi_2}\right]/\alpha \quad \text{for symmetric modes}. \tag{11}$$

The resonant frequency for IF modes can be obtained from the relation $\xi_1\equiv\xi_2$. For a wurtzite FSQW, as before, ξ_2 must be replaced by 1. In the absence of dielectric anisotropy, Eq. (11) transforms to the dispersion relation known for zinc-blende QW's.[3]

C. Propagating modes

Overlapping of the characteristic phonon frequencies creates conditions for the appearance of so-called propagating (P) modes for which the requirement of Eq. (6a) must be satisfied in both media. In the absence of damping, however, the BC of Eq. (7) cannot be applied for a given case. Nevertheless, to obtain the dispersion relation for the propagating modes we can use an additional requirement. In the absence of retardation, it can be shown that the propagating extraordinary waves obey the condition $-\vec{\kappa}\times\vec{E}=0$.[4]

The chosen symmetry of the problem leads to

$$\kappa_z\frac{\partial\Phi(r)}{\partial\rho}-q\frac{\partial\Phi(r)}{\partial z}=0. \tag{12}$$

Then, the BC for the tangential component of the electric field can be rewritten as

$$\frac{1}{2\beta}\frac{\partial\Phi_2(z)}{\partial z}\bigg|_{z=\mp d/2}-\frac{1}{2\alpha}\frac{\partial\Phi_1(z)}{\partial z}\bigg|_{z=\mp d/2}=0, \tag{13}$$

where $\beta=\frac{1}{2}\sqrt{|\epsilon_{2t}(\omega)/\epsilon_{2z}(\omega)|}$. From Eqs. (2) and (3), the potentials in media 1 and 2 are found to be

$$\Phi_1(z)=A\cos(2\alpha Q_m z/d)+B\sin(2\alpha Q_m z/d), \tag{14}$$

and

$$\begin{aligned}\Phi_2(z)=&\left[\pm\left(\mu\frac{\xi_1}{\xi_2}\cos(\beta Q)\sin(\alpha Q)-\cos(\alpha Q)\sin(\beta Q)\right)A\right.\\&+\left(\mu\frac{\xi_1}{\xi_2}\cos(\beta Q)\cos(\alpha Q)\right.\\&\left.\left.+\sin(\beta Q)\sin(\alpha Q)\right)B\right]\sin(2\beta Q z/d)\\&+\left[\left(\mu\frac{\xi_1}{\xi_2}\sin(\alpha Q)\sin(\beta Q)+\cos(\alpha Q)\cos(\beta Q)\right)A\right.\\&\pm\left(\mu\frac{\xi_1}{\xi_2}\cos(\alpha Q)\sin(\beta Q)\right.\\&\left.\left.-\sin(\alpha Q)\cos(\beta Q)\right)B\right]\cos(2\beta Q z/d),\end{aligned} \tag{15}$$

where the upper (lower) signs correspond to negative (positive) z. With this result, Eq. (13) can be transformed into the following system of equations:

$$\chi(A\sin(\alpha Q)+B\cos(\alpha Q))=0,$$
$$\chi(-A\sin(\alpha Q)+B\cos(\alpha Q))=0, \tag{16}$$

with

$$\chi=1-\mu\frac{\xi_1}{\xi_2}. \tag{17}$$

The condition $\chi=0$ corresponds to the dispersionless solution $\omega=\omega'$. At this ''frequency of transparency'' waves with any values of $q>0$ will ''propagate'' through the QW.

Finally, the dispersion relation for propagating modes reduces to

$$Q_{m'}=\frac{m'\pi}{2\alpha} \quad \text{for} \quad \omega\neq\omega' \tag{18}$$

with $m'=1,3,5,\ldots$ for antisymmetric modes and $m'=2,4,6,\ldots$ for symmetric modes.

These results are as expected. From the collinearity requirement for $\vec{\kappa}$ and $\vec{E}$ and the BC's for E_t and D_z, it follows that at an interface

$$\frac{\kappa_{2z}}{\kappa_{1z}}=\mu\frac{\epsilon_{1z}(\omega)}{\epsilon_{2z}(\omega)}, \tag{19}$$

which, for $\mu=1$, immediately yields the condition $\chi=0$, since $\kappa_z=\sqrt{\epsilon_t(\omega)/\epsilon_z(\omega)}q$. The frequency of a P mode can differ from ω' if and only if the condition $\partial\Phi_1(z)/\partial z|_{z=\mp d/2}=\partial\Phi_2(z)/\partial z|_{z=\mp d/2}=0$ is satisfied, i.e., when the z component of the electric field vanishes at the interface providing for the fulfillment of both BC's and collinearity independently of the z components of the dielectric tensor. In that case, the solution is given by Eq. (18).

In QW's made from isotropic materials there are no P modes defined above. Indeed, substituting $\xi_1\to\epsilon_1(\omega)$, $\xi_2\to\epsilon_2(\omega)$ in Eq. (16) we find that the only possible solution would correspond to the case if $\epsilon_1(\omega_{LO})=\epsilon_2(\omega_{LO})=0$, i.e., when the materials 1 and 2 are identical. The only exception is for the hypothetical case, which would correspond to either different TO frequencies in both materials or coincidence of the LO frequencies of one (or more) modes in heterostructures made of materials with multimode behavior of the phonon branches.

D. Half-space modes

We define half-space modes as the modes that should satisfy the conditions of Eqs. (6b) and (6a) in media 1 and 2, respectively. This definition is dictated by the fact that conditions $\Phi_2(\pm d/2)=0$ and $\partial\Phi_2(z)/\partial z|_{z=\mp d/2}=0$ must be excluded from consideration because in both these cases the BC's can be satisfied only for $q\equiv 0$.

General solutions in media 1 and 2 can be represented as

$$\Phi_1(z)=A\cosh(2\alpha Q z/d)+B\sinh(2\alpha Q z/d),$$
$$\Phi_2(z)=a\cos(2\beta Q z/d)+b\sin(2\beta Q z/d). \tag{20}$$

TABLE I. Material parameters.

Material	ω_{Lz} (cm^{-1})	ω_z (cm^{-1})	ω_{Lt} (cm^{-1})	ω_t (cm^{-1})	ϵ^{∞}
GaN[a]	735	533	743	561	5.29
AlN[a]	893	660	916	673	4.68
$Al_{0.15}Ga_{0.85}N$[b]	772	544	783	570	5.20[c]

[a]Reference 6.
[b]Reference 7.
[c]The value of ϵ^{∞} fot the ternary compound was estimated by the linear interpolation.

Applying the BC's of Eq. (3) for these potentials and taking into account that for symmetric (antisymmetric) solution both coefficients B and b (A and a) are equal to zero we found the dispersion relations for HS modes to be

$$\beta Q_m^a - \mu \arctan\left[\frac{\xi_2}{\xi_1}\tanh(\alpha Q_m^a)\right] - m\pi = 0$$

for antisymmetric modes, (21)

$$\beta Q_m^s + \mu \arctan\left[\frac{\xi_1}{\xi_2}\tanh(\alpha Q_m^s)\right] - m\pi = 0$$

for symmetric modes.

In Eq. (21), $m = 1,2,3,4\ldots$ and 0 for the cases when a solution $Q_0(\omega) \neq 0$ can exist in any of the allocated frequency intervals.

The HS modes in a heterostructure formed by optically isotropic media are the oscillatory waves in medium 2 with zero potential at the interfaces. This implies no optical vibrations inside of the QW. The latter circumstance makes it impossible to obtain the dispersion relation in terms of parameters of the QW: α, d, and $\epsilon_1(\omega)$. Therefore, the anisotropy of the dielectric media provide unique possibilities to influence the dispersion of HS modes varying the appropriate parameters of the QW.

IV. POLAR MODES IN NITRIDE-BASED HETEROSTRUCTURES: DISCUSSION

Compared to the dielectrically isotropic case, a few significant peculiarities appear in the optical phonon spectra. The main source of these peculiarities is the inseparable relation between the phonon wave number and its frequency given by condition of Eq. (5). This relation together with the BC's determine the behavior of the polar phonon modes in finite energy intervals defined by characteristic phonon frequencies. Since the energy intervals allocated to each of the types of phonon modes can be regulated by composition variations, investigation of the effect of these variations on phonon spectra is very important for understanding of phonon-related processes in wurtzite-based heterostructures. In this section, we illustrate peculiarities of composition-dependent phonon spectra in wurtzite low-dimensional structures for the example of AlN/GaN-based QW's.

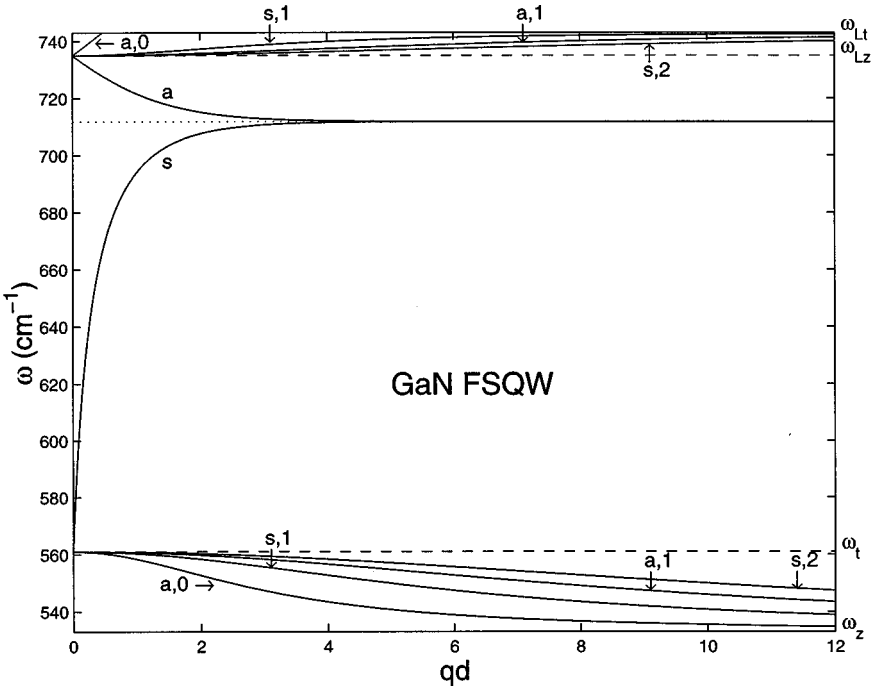

FIG. 1. Dispersion of the polar optical phonons in GaN FSQW. Only four confined modes are shown in each interval. The modes are identified according to both symmetry and quantum number. The characteristic frequencies are shown by the dashed lines. The dotted line indicates resonant frequency for the IF mode.

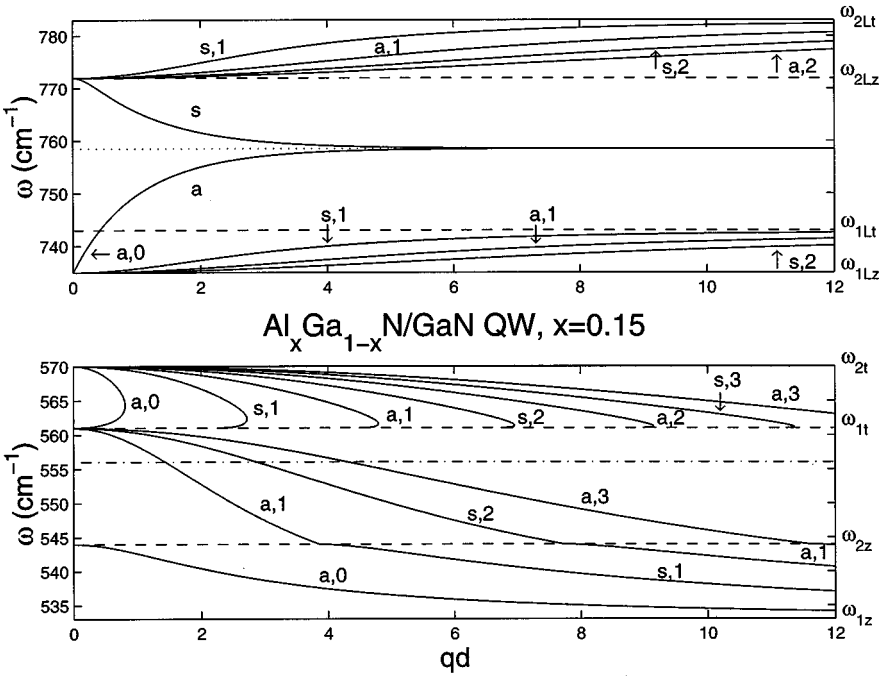

FIG. 2. Dispersion of the polar optical phonons in a ternary-binary system. Only a few confined, propagating, and half-space modes are shown in each corresponding interval. The modes are identified according to both symmetry and quantum number. The characteristic frequencies are shown by the dashed lines. The dotted line indicates the resonant frequency for the IF_{II} mode. The dot-dashed line indicates the frequency of transparency ω'.

Parameters of the materials are given in Table I. The values of composition-dependent characteristic frequencies at $x=0.15$ were estimated taking into account the one-mode behavior of the polar modes in $Al_xGa_{1-x}N$.[8] Dispersion curves for the optical phonon modes in a GaN dielectric slab and an $Al_xGa_{1-x}N/GaN/Al_xGa_{1-x}N$ QW with $x=0.15$ are shown on Figs. 1 and 2, respectively. Since at $x=1$ the dispersion in interval $\omega\in[\omega_{2t}\cdots\omega_{2Lt}]$ is qualitatively the same as in case of $x=0.15$, only the low-energy optical phonon modes in AlN/GaN/AlN QW are shown on Fig. 3.

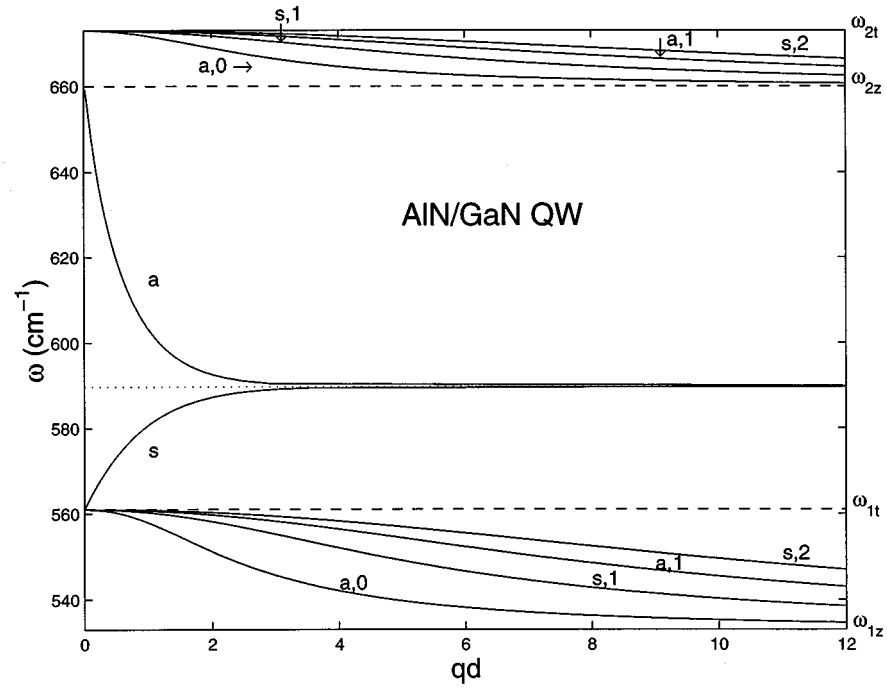

FIG. 3. Low-energy part of the dispersion of the polar optical phonons in AlN-GaN QW. Only a few confined, and half-space modes are shown in each corresponding interval. The modes are identified according to both symmetry and quantum number. The characteristic frequencies are shown by the dashed lines. The dotted line indicates resonant frequency for the IF_I.

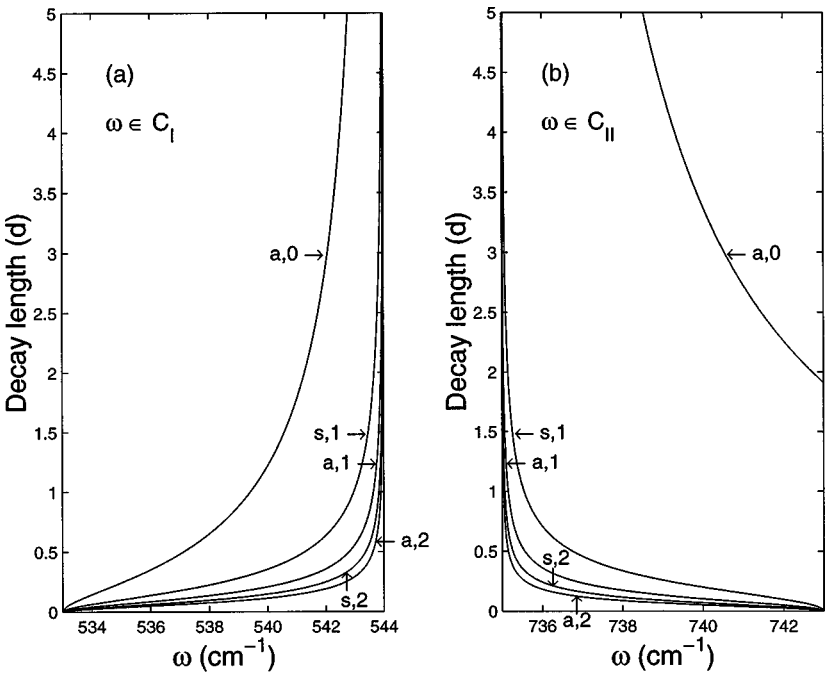

FIG. 4. Degree of confinement for the confined modes with $m \leqslant 2$: (a) interval C_I; (b) interval C_{II}. The modes are identified according to both symmetry and quantum number.

For a symmetrical AlN/GaN/AlN QW as well as for a GaN FSQW, C modes exist in *two* frequency intervals $[\omega_{1z} \cdots \omega_{1t}]$ (C_I) and $[\omega_{1Lz} \cdots \omega_{1Lt}](C_{II})$. However, it follows from the composition-dependent Raman shift of the characteristic frequencies of infrared active modes in ternary $Al_xGa_{1-x}N$ compounds[7–9] that at appropriate values of x the ternary-binary system exhibits the peculiar feature of overlapping TO-like frequency intervals $[\omega_z \cdots \omega_t]$. Due to this overlap, the interval C_I reduces to $[\omega_{1z} \cdots \omega_{2z}]$ as shown in Fig. 2.

In a wurtzite heterostructure, the wave vector of the confined phonons becomes frequency dependent; i.e., it is characterized by appropriate dispersion. In the interval C_I (C_{II}), the antisymmetric modes with $m=0$ correspond to the lowest (highest) energy at a given q. The quantum number m can take any integer value (and zero for the antisymmetric mode) for both symmetric and antisymmetric modes. Confinement of the modes is characterized by leakage of the potential from the QW and depends strongly on the frequency. This dependence is illustrated on Fig. 4 where the decay length in medium 2 is taken as a measure of confinement. As shown on Fig. 4, confinement of the modes of higher order is much stronger with respect to the modes with $m=0$ and increases with increasing q for all the modes. At the same time, compared to the mode with $m=0$ in the interval C_{II}, the lowest mode in the interval C_I manifests significantly stronger localization.

The mode $m=0$ in the interval C_{II} exhibits unique behavior. At the resonant frequency $\omega^{res}=\omega_{1tL}$, this mode has a finite value of $q=(2/d)\epsilon_{1z}(\omega_{1tL})/\xi_2(\omega_{1tL})$ (with $\xi_2 \equiv 1$ for the case of FSQW) and the highest energy among all the other confined modes. In an embedded QW and at the same resonant frequency this mode transforms to the antisymmetric IF mode. As shown on Fig. 4, a finite value of the wave vector as well as absence of singularities in ϵ_{2t}^{-1} and ϵ_{2z} at the resonant frequency implies reduced localization for this mode compared to all the other modes as $\omega \to \omega^{res}$.

Shrinking of the region C_I, induced by the composition-dependent frequency overlap, leads to discretization of the wave vector $\vec{q}$ at the frequency ω_{2z}. At this frequency, symmetric, with $q_m=\pi(m-1/2)/\alpha(\omega_{2z})$, and antisymmetric, with $q_m=\pi m/\alpha(\omega_{2z})$, C modes $(m=1,2,3\ldots)$ transform into the antisymmetric, with $m'=1,3,5\ldots$, and symmetric, with $m'=2,4,6\ldots$, propagating modes, respectively. It should be pointed out that although at ω_{2z} the wave numbers of all C modes with $m>0$ are finite, the decay length in this case is infinite since $\epsilon_{2z}(\omega_{2z})^{-1} \equiv 0$.

In a wurtzite dielectric slab, two IF modes exist in the frequency interval $[\omega_{1t} \cdots \omega_{1Lz}]$. At the same time, the AlN/GaN/AlN QW would manifest *four* interface modes.[10] Two pairs of modes are found in two frequency intervals: $[\omega_{1t} .. \omega_{2z}]$ (IF_I) and $[\omega_{1tL} \cdots \omega_{2zL}]$ (IF_{II}). For the case of $x=0.15$, however, the relation $\omega_{2z} < \omega_{1t}$ is satisfied so that inverted interval IF_I now corresponds to the propagating modes. As a result, only *two* IF modes located in the interval IF_{II} can exist for such a heterostructure. The values of resonant frequencies are 711.8 and 758.5 cm^{-1} for the slab and ternary-binary system, respectively. At $x=1$, these frequencies are approximately 589.7 cm^{-1} (interval IF_I) and 838.4 cm^{-1} (interval IF_{II}).

It should be emphasized that although the condition of Eq. (6b) is satisfied for $\omega \in [\omega_{2t} \cdots \omega_{1Lz}]$, no polar modes can exist in this frequency interval since the z components of the dielectric tensor have the same sign in both media. In fact, this feature of the ternary-binary wurtzite heterostructures allows the formation of relatively wide composition-dependent energy gaps (around 8 meV at $x=1$ and 21 meV at $x=0.15$) forbidden for the polar optical oscillations. One can expect that the appearance of such gaps in optical-phonon spectra should influence scattering processes in the QW, especially when the characteristic energy of the electron transitions is of the order of the width of a phonon-free band.

Note that in the case shown on Fig. 2, two IF modes exist in a quite narrow energy interval and are characterized by

low values of group velocity. At the same time, the energy interval occupied by the IF modes in the GaN FSQW is much wider and the strong dispersion of the symmetric mode in the long-wavelength range suggests that the IF phonons in the FSQW conduct more energy along the well. In general, for the given system, an increase in x leads to redistribution of the energy transferred by IF phonons so that at higher values of x the antisymmetric modes become the main energy carriers.

Besides the narrowing of the interval C_I which is accompanied by limitation of the lowest allowed q values with $m>0$ and the decrease in the number of IF modes, the overlap of the characteristic frequencies leads to the appearance of propagating modes in the optical phonon spectrum at $\omega \in [\omega_{2z} \cdots \omega_{1t}]$. As shown on Fig. 2, P modes are characterized by a dispersive quantized spectrum where at each particular energy, the state with the lowest q corresponds to the antisymmetric mode with $m'=1$. Quantization of the spectrum is caused by the requirement of collinearity for the phonon wave vector and the electric field for the waves propagating in uniaxial crystal under conditions when retardation effects can be neglected. This requirement implies an extremum in the phonon potential at the interfaces for almost all the frequencies where the propagating modes can exist. An exception is the ''frequency of transparency,'' ω', indicated by the dot-dashed line in Fig. 2. At this particular frequency, which can be estimated as $\omega' \approx 556.05\ \mathrm{cm}^{-1}$ for the case represented on Fig. 2, waves with arbitrary q can ''propagate'' through the QW. For phonons oscillating with frequency, ω', the product $\kappa_z \epsilon_z$ is invariant. It is worth noting that conditions for the existence of such dispersionless waves can be satisfied only for positive μ.

When the characteristic frequencies of each medium are separated in energy, the HS modes exist in two intervals: HS_I $(\omega \in [\omega_{2z} \ldots \omega_{2t}])$ and HS_{II} $(\omega \in [\omega_{2zL} \ldots \omega_{2tL}])$. If a frequency overlap occurs, the interval HS_I reduces to $[\omega_{1t} \ldots \omega_{2t}]$. The HS modes also manifest very specific behavior. Contrary to the isotropic case, in wurtzite heterostructures the dispersion relation for these modes can be obtained in terms of the parameters of the QW. Due to penetration of the HS phonons into the QW, the modes are expected to have much stronger effect on the scattering processes. Like C modes, the HS modes exist in *two* energy intervals. They are dispersive and quantized. However, the lowest, in terms of quantum number m, HS modes in the intervals HS_I and HS_{II} have different symmetry: the antisymmetric mode with $m=0$ is absent in the interval HS_{II}. This peculiarity also holds at $x=1$.

As follows from the dispersion relation of Eq. (21), the frequency overlap leads to discretization of the q values at frequency ω_{1t} according to the relations $Q=m\pi/\beta(\omega_{1t})$ for antisymmetric modes and $Q=\pi(m-1/2)/\beta(\omega_{1t})$ for symmetric modes. As a result, dispersion of the long-wavelength HS phonons in the interval HS_I dramatically increases. This peculiarity opens the way to influence strongly the group velocity of these modes by variation of the composition.

Except for the IF and dispersionless P modes, the existence of the appropriate phonon modes in a given interval is independent on μ. It is interesting, however, that the value of this parameter can determine the symmetry of a particular mode. This, in turn, can strongly influence the electron-phonon interaction at given energy.

Finally, the analysis made in this section leads to the conclusion that the features of the wurtzite-based heterostructures, as well as the dependence of these features on composition, gave rise to new possibilities for phonon spectrum engineering in various optoelectronic applications.

V. SUMMARY

We have considered spectra of the optical phonons in wurtzite QW's for the case when the optical axis is parallel to the interface. These spectra manifest a number of features caused by the anisotropy of the dielectric properties of the media as well as the composition-dependent overlap of characteristic phonon frequencies of the QW and the surrounding material. It is found, that contrary to the case of QW's made of cubic crystals, confined and half-space modes are dispersive and characterized by the leakage of the potential through the interfaces. The depth of the potential tails strongly depends on frequency and the order of a given mode, so that spatial localization of the long-wavelength phonons is very weak. The symmetry of a mode is determined by the signs of z components of the dielectric tensors in both media. Overlap in characteristic frequencies reduces the number of interface modes, strongly influences the dispersion of HS and C modes, and leads to the appearance of dispersive and dispersionless propagating modes with frequency of transparency determined by conservation of the quantity $\epsilon_t \epsilon_z$.

The predicted existence of the ''frequency of transparency,'' the dispersive nature of propagating, half-space and weakly localized confined modes, as well as the composition-dependent width of the intervals where particular modes can exist, appearance of forbidden gaps for the polar optical vibrations, and variation of phonon-assisted energy transport along the QW are some of the unique features of phonons in confined wurtzite systems that have not yet been observed experimentally. These features portend many interesting applications of confined wurtzite semiconductor structures in both optoelectronic and electronic technology.

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