Energy-dependent electron scattering via interaction with optical phonons in wurtzite crystals and quantum wells

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A formalism for the calculation of the scattering rate in wurtzite-type crystals and quantum wells (QW's) is developed taking into account features of the optical phonon spectra in an optically anisotropic medium. The electron-scattering rate due to the interaction with infrared/Raman-active polar optical phonons in GaN, bulk material, and heterostructures, is investigated. To determine the dependence of scattering rate on optical anisotropy and dimensionally induced transformation of the phonon spectra, three cases are considered: (a) bulk material with different orientations of the electron wave vector with respect to the optical axis; (b) a system in which bulk phonons interact with electrons confined in a QW; and (c) free-standing and embedded QW's where the effects of confinement of both electron and phonon subsystems are taken into account. It is found that the scattering rate depends weakly on the initial orientation of the electron wave vector. Exceptions are the energy intervals which correspond to the threshold values for emission of both TO-like and LO-like bulk phonons. Our results reveal a complex and strong dependence of the electron-scattering rate on the dispersion of a particular mode. Moreover, this dependence is found to be the main factor which determines electron-phonon scattering in wurtzite heterostructures, in particular, through the relation between phonon phase and group velocities. For the optically anisotropic media considered, the effect of spatial localization of the phonon modes on the scattering rate is found to be as strong as the effect of electron confinement.

I. INTRODUCTION

Recent interest in nitrides has been stimulated by the discovery of blue and green high power GaN-based light emitters[1,2] as well as by attempts to utilize the unique properties of the nitrides, such as the ability to operate at high temperatures,[3] high frequency, and high power density.[4,5] At room and higher temperatures, the main mechanism that influences electron transport is anticipated to be scattering by polar optical phonons.[6] Indeed, one can expect that the scattering processes will be strongly influenced by high-energy optical phonon modes over a wide range of temperatures since GaN is characterized by a relatively large gap which separates the optical and acoustic branches.[7] On the other hand, the theory of charge scattering by optical modes in uniaxial crystals, such as wurtzite GaN, has not yet been adequately developed.

The main results known in the theory of electron-phonon interaction were obtained for the case of optically isotropic materials due to the relative simplicity of their phonon spectra. Nitrides of Ga and Al, however, are usually crystallize in the hexagonal wurtzite structure (space group C_{6v}^4). The unit cell in such a material contains four atoms. Consequently, there are nine optical-phonon branches. Only two branches are both Raman and infrared active. They correspond to the extraordinary A_1 and E_1 modes in irreducible representation at the Γ point. Since wurtzites have a special (optical) axis along which plane electromagnetic waves propagate with a velocity independent of the direction of their polarization vector, they belong to the family of so-called uniaxial crystals. In wurtzites, the optical axis coincides with the c axis which is perpendicular to the hexagons. Due to the optical anisotropy of uniaxial crystals, the long-wavelength lattice vibrations can be classified according to mutual orientation between the c axis, the phonon wave vector $\mathbf{q}$, the electric field $\mathbf{E}$, and the polarization $\mathbf{P}$.[8] This classification divides the lattice vibrations into two groups of phonons, ordinary and extraordinary. In the no-retardation limit, the ordinary phonons, for which, in general, $\mathbf{E}$ and $\mathbf{P}$ are both perpendicular to $\mathbf{q}$ and the c axis, become dispersionless and have zero electric vector. At the same time, frequencies of extraordinary phonons become dependent exclusively on the angle θ between the phonon wave vector and the optical axis. For these phonons $\mathbf{q} \| \mathbf{E}$ and $\mathbf{E} \neq 0$ for $\theta \neq 0, \pi/2$. The extraordinary A_1 and E_1 modes split into LO and TO components. The pure A_1 phonon is polarized in the direction of the c axis and the pure E_1 phonon is polarized in the normal plane. For arbitrary θ, however, the extraordinary phonon would exhibit a mixed polarization. It is obvious, therefore, that the phonon spectra in wurtzites are far more complicated than those of cubic crystals and have to be taken into account explicitly when considering the electron-phonon interaction. Indeed, even in bulk crystals, inherent optical anisotropy leads to finite interaction of electrons with transverselike phonon branches depending on the orientation of both electron and phonon momenta with respect to the c axis.[9] Recently,[10] it has been found that due to the directional dependence of the components of the permittivity tensor in wurtzites, the phonon spectra in nanostructures differ qualitatively from those observed in cubic quantum hetero-

structures and are characterized by phenomena including the absence of proper confinement of the phonon modes; strong dispersion of not only interface (IF) but also confined and half-space modes; and composition-dependent symmetry and the number of particular modes. Nevertheless, the influence of all these features of the phonon spectra in wurtzites on transport phenomena had not yet been investigated.

In the present paper, we explicitly include the peculiarities of the phonon spectra obtained in the framework of the dielectric continuum model into consideration of electron scattering in wurtzites and investigate the angle and energy dependence of electron–optical-phonon scattering in bulk GaN as well as the influence of spatial confinement of both electron and phonon subsystems on the electron transition frequency. In doing so, we take advantage of Loudon's uniaxial crystal model[8] and the macroscopic dielectric continuum approach. The scattering rates are obtained in the first Born approximation.

II. SCATTERING RATE

A. Bulk materials

In wide-gap semiconductors such as GaN, electron-phonon interactions take place at relatively high values of phonon wave vectors $\mathbf{q}$ so that the relation $qc_l \gg \omega$ (here c_l is the speed of light) is satisfied for all optical frequencies ω. For these conditions, the retardation effects can be neglected and dependence of the phonon frequencies on θ can be represented as

$$\epsilon_t(\omega)\sin^2\theta+\epsilon_z(\omega)\cos^2\theta=0, \tag{1}$$

where

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

The subscripts z an t denote the directions parallel and perpendicular to the c axis; ω_{Lz}, ω_z, ω_{Lt}, and ω_t are the characteristic frequencies of the A_1(LO),A_1(TO),E_1(LO), and E_1(TO) modes, respectively. We also assume that $\epsilon_z^{\infty}\approx\epsilon_t^{\infty}=\epsilon^{\infty}$.

General consideration of the scattering in wurtzite crystals indicates that it is sufficient to choose the initial electron wave vector in the y-z plane with the z axis oriented along the optical axis c. Then, using the interaction Hamiltonian derived previously,[9,11] the scattering rate can be expressed as

$$\frac{1}{\tau_e^{(a)}}=\frac{1}{\pi a_B}\sqrt{\frac{m^*\hbar}{2m_0}}\int_0^{\pi}\frac{\left(N+\frac{1}{2}\mp\frac{1}{2}\right)\sin\theta}{\sqrt{\omega\left[\frac{\partial\epsilon_t}{\partial\omega}\sin^2\theta+\frac{\partial\epsilon_z}{\partial\omega}\cos^2\theta\right]}}$$

$$\times\int_0^{2\pi}\frac{\sigma}{\sqrt{\frac{E_k}{\hbar\omega}\cos^2\widehat{\mathbf{kq}}\pm 1}}\,d\phi\,d\theta, \tag{2}$$

where upper (lower) signs correspond to the processes accompanied by absorption (emission) of the phonons, $\cos\widehat{\mathbf{kq}}=\sin\theta\sin\theta_k\sin\phi+\cos\theta\cos\theta_k$, θ_k is the angle between the initial electron wave vector $\mathbf{k}$ and the c axis, ϕ is the azimuthal angle in plane perpendicular to the z axis, ω is the solution of the relation $\cos^2\theta=\epsilon_t(\omega)/[\epsilon_t(\omega)-\epsilon_z(\omega)]$, a_B is the radius of the first Bohr electron orbit, N is the phonon occupation number, m^* is the dimensionless effective mass of the electron with mass m_0, and σ is a step function defined as

$$\sigma=\begin{cases}0 & \text{for } \cos(\widehat{\mathbf{kq}})<\sqrt{\hbar\omega/E_k},\\ 2 & \text{otherwise.}\end{cases} \tag{3}$$

For processes involving absorption of phonons, $\sigma\equiv 1$. As a final and parenthetical comment in this subsection, Eq. (2) extends the result obtained previously[9] since it can be applied for arbitrary relationships between the characteristic frequencies.

B. Quantum wells

In this subsection, we consider the scattering of electrons with a symmetric wave function which corresponds to the ground state in a quantum well (QW) of width d. We assume that the z axis is collinear with the optic axis and perpendicular to the heterointerfaces. The origin of the coordinates is located at the geometrical center of the well. With these assumptions, the dispersion relations for the symmetric confined and IF modes are given by[10]

$$q=[n\pi+\mu\arctan(\xi_2/\xi_1)]/(\alpha d)$$
$$(n=1,2,3\ldots \text{ and } 0 \text{ if } \mu=1), \tag{4}$$

and

$$q=\frac{1}{2}\ln\left[\frac{\xi_1+\xi_2}{\xi_1-\xi_2}\right]\Big/(\alpha d), \tag{5}$$

respectively. Here q is the magnitude of two-dimensional phonon wave vector, $\mu=\text{sign}[\epsilon_{1z}(\omega)\epsilon_{2z}(\omega=)]$, ξ_1 $\xi 1=\sqrt{|\epsilon_{1z}(\omega)\epsilon_{1t}(\omega)|}$, $\xi_2=\sqrt{|\epsilon_{2z}(\omega)\epsilon_{2t}(\omega)|}$, and α $\alpha=\frac{1}{2}\sqrt{|\epsilon_{1,t}(\omega)/\epsilon_{1,z}(\omega)|}$. Indices 1 and 2 are related to the QW and surrounding materials, respectively. The normalization condition for the orthogonal modes in a wurtzite QW is

$$\int\left(\frac{\partial\epsilon_t}{\partial\omega}|\mathbf{E_t}|^2+\frac{\partial\epsilon_z}{\partial\omega}|\mathbf{E_z}|^2\right)dz=\frac{4\pi\hbar}{L_xL_y}. \tag{6}$$

Then, in terms of notation defined previously, the Hamiltonians for the interaction of an electron with confined phonons, H^C, and with IF phonons, H^{IF}, become

$$H^C=\sum_{q_n}\left[\frac{4\pi\hbar e^2(q_nL_xL_y)^{-1}}{\cos^2(\alpha q_n d)\zeta^+(\beta)+\alpha q_n d\zeta^+(\alpha)+\cos(\alpha q_n d)\sin(\alpha q_n d)\zeta^-(\alpha)}\right]^{1/2}$$

$$\times e^{i\mathbf{q}\rho}(a_q+a^\dagger_{-q})\begin{cases}\cos(2\alpha q_n z) & |z|\leqslant d/2\\ \cos(\alpha q_n d)e^{\beta q_n d(1-2|z|/d)} & |z|>d/2,\end{cases} \tag{7}$$

and

$$H^{IF}=\sum_{q}\left[\frac{4\pi\hbar e^2(qL_xL_y)^{-1}}{\cosh^2(\alpha qd)\zeta^+(\beta)+\alpha qd\zeta^-(\alpha)+\sinh(\alpha q_n d)\zeta^+(\alpha)/2}\right]^{1/2}$$

$$\times e^{i\mathbf{q}\rho}(a_q+a^\dagger_{-q})\begin{cases}\cosh(2\alpha q_n z) & |z|\leqslant d/2\\ \cosh(\alpha q_n d)e^{\beta q_n d(1-2|z|/d)} & |z|>d/2,\end{cases} \tag{8}$$

respectively. Here ρ is the radius vector in the x-y plane, $\zeta^\pm(x)=(1/2x)(\partial\epsilon_{jt}/\partial\omega)\pm 2x(\partial\epsilon_{jz}/\partial\omega)$, $\beta=\frac{1}{2}\sqrt{|\epsilon_{2,t}(\omega)/\epsilon_{2,z}(\omega)|}$, e is the elementary charge, a_q and $a^\dagger_{-q}$ are the annihilation and creation operators, respectively. The index j takes on the value of 1 if $x=\alpha$ and the value 2 otherwise. Taking into account the dispersion relations, the corresponding squared matrix element $|M^{(C}_{IF)}|^2$ can be expressed as

$$|M^{(C}_{IF)}|^2=\frac{4\pi\hbar e^2}{qL_xL_y}D(q,\omega)^{(C}_{IF)}\left(N+\frac{1}{2}\mp\frac{1}{2}\right)\delta_{k-k'\pm q}, \tag{9}$$

with

$$D(q,\omega)^{(C}_{IF)}=\frac{\left[\dfrac{\Upsilon^2}{\alpha^2q^2\mp k_1^2}\left\{\left(\dfrac{k_1^2\mp\alpha^2q^2}{k_2+\beta q}\xi_1-\alpha q\mu\xi_2\right)\cos^2\left(\dfrac{1}{2}dk_1\right)\pm\dfrac{\mu k_1^2\xi_2}{2\alpha q}+\dfrac{1}{2}\sin(dk_1)k_1\xi_1\right\}\right]^2}{\zeta^\pm(\alpha)dq\alpha(\xi_1^2\pm\xi_2^2)\pm\zeta^\mp(\alpha)\mu\xi_1\xi_2+\zeta^+(\beta)\xi_1^2}. \tag{10}$$

In Eq. (10), upper (lower) signs must be taken when considering electron interaction with C (IF) modes; k_1 and k_2 are the magnitudes of the lateral components of the electron wave vector inside and outside the QW, respectively; Υ is the amplitude of the electron wave function:

$$\Upsilon=[\sin(k_1d)/(2k_1)+d/2+\cos^2(k_1d/2)/k_2]^{-1/2}. \tag{11}$$

At this point, we emphasize two important peculiarities which make consideration of electron–optical-phonon scattering in wurtzite QW's different from the case of an optically isotropic material.[12] As follows from the matrix element given previously in this paper, it is impossible to derive a pure form factor for the system under consideration. The inherent anisotropy of the dielectric medium leads to the leakage of the phonon potential of all modes from the QW (Ref. 10) and mixing of longitudinal and lateral phonon momenta. As a result, the ''form factor'' represented in the numerator of Eq. (10) becomes dependent on the parameters of both subsystems. Another significant consequence of the low wurtzite symmetry is the dispersive character of the confined phonons. In addition, IF phonon modes in a wurtzite free-standing QW may also exhibit strong dispersion. These features suggest that, in general, the relationship between the phonon momentum and frequency has to be taken into account explicitly when deriving the scattering rate from the Fermi golden rule. One can perform this as follows. For a particular mode, we define $P=P(q,\omega)=(N+\frac{1}{2}\mp\frac{1}{2})D(q,\omega)$ and $L=L(q,\omega,\theta)=(E_{\mathbf{k}\pm\mathbf{q}})-E_{\mathbf{k}}\mp\hbar\omega$. Then

$$\begin{aligned}1/\tau&\propto\int P/q\,\delta(L)d\mathbf{q}\\ &=\int P\,\delta(L)dqd\theta\\ &=\int P\left|\frac{dL}{dq}\right|^{-1}d\theta=\int P\left|\frac{dL}{dq}\right|^{-1}\left|\frac{d\theta}{d\omega}\right|d\omega.\end{aligned} \tag{12}$$

Applying this set of transformations and using momentum conservation to eliminate the $k\cos\theta$ term from the denominator as well as to obtain derivatives $d\theta/d\omega$, the scattering rate can be expressed as

$$\frac{1}{\tau_e^{(a)}}=\frac{2m^*}{a_B}\sum_{n=(1-\mu)/2}\int_{\omega_1}^{\omega_2}\frac{\left(N+\frac{1}{2}\mp\frac{1}{2}\right)D(q,\omega)\left[\left(\frac{V_{ph}}{q}\pm\frac{\hbar}{2m^*m_0}\right)\frac{1}{V_{gr}}-\frac{1}{q}\right]}{\left(\frac{q}{2}\pm\frac{m^*m_0}{\hbar}[V_{ph}-V_{gr}]\right)\sqrt{\frac{1}{m^*m_0}\left(2E_k-\frac{1}{2}E_q\pm\hbar\omega\right)-V_{ph}^2}}d\omega, \tag{13}$$

where V_{ph} and V_{gr} are the phonon phase and group velocities, respectively, and $E_q=\hbar^2q^2/(2m^*m_0)$. The integration limits must be determined from the relations

$$\frac{m^*m_0\omega}{kq\hbar}-\frac{q}{2k}=\pm1 \quad \text{for absorption,}$$
$$\frac{m^*m_0\omega}{kq\hbar}+\frac{q}{2k}=1 \quad \text{for emission.} \tag{14}$$

Phonon emission starts when the electron energy reaches the value $\hbar\omega_{\min}$ where $\omega_{\min}$ is determined from the relation $q=\sqrt{2m^*m_0\omega/\hbar}$. For the case of IF modes, the summation over n should be omitted.

To elucidate the effect of phonon mode confinement on the scattering of carriers with wave functions completely localized in the QW, we have also calculated the scattering rate for the case when the phonon modes have bulk dispersion. Since, as will be shown subsequently, the angle dependence for the bulk electron-phonon system is weak, this effect can be estimated using arbitrary system configuration. To obtain analytical expressions for τ^{-1}, a configuration with the c axis perpendicular to the heterointerface will be assumed.

The square of the matrix element for such a system has the form

$$|M|^2=\frac{16\pi e^2\hbar}{Vq^2d^2\left[\frac{\partial\epsilon_t}{\partial\omega}\sin^2\theta+\frac{\partial\epsilon_z}{\partial\omega}\cos^2\theta\right]}\times\left(\frac{4\pi^2\sin\left(\frac{d}{2}q\cos\theta\right)}{(4\pi^2-(dq\cos\theta)^2)q\cos\theta}\right)^2\times\left(N+\frac{1}{2}\mp\frac{1}{2}\right)\delta_{k-k'\pm q}, \tag{15}$$

where V is the characteristic volume and $q\cos\theta$ represents the z component of three-dimensional phonon wave vector $\mathbf{q}$. Then, the scattering rate is

$$\frac{1}{\tau_e^{(a)}}=\frac{64\pi^3m^*}{a_Bd^2}\int_0^{\pi}\frac{\left(N+\frac{1}{2}\mp\frac{1}{2}\right)\tan\theta}{\cos\theta\left[\frac{\partial\epsilon_t}{\partial\omega}\sin^2\theta+\frac{\partial\epsilon_z}{\partial\omega}\cos^2\theta\right]}\times\int_0^{2\pi}\frac{\sigma_1F(q)^{(a)}_{(e)}}{\sqrt{\chi^2_{\theta,\phi,k_\parallel}\pm\frac{2m^*m_0\omega}{\hbar}}}d\phi d\theta, \tag{16}$$

with

$$F(q)=\frac{\sin^2\left(q\frac{d}{2}\cos\theta\right)}{q^2(4\pi^2-q^2d^2\cos^2\theta)^2} \tag{17}$$

and

$$F^{(a)}_{(e)}=\begin{cases}F(q_a) & \text{for absorption,}\\ (F(q_{e^-})+F(q_{e^+}) & \text{for emission,}\end{cases} \tag{18}$$

where

$$q_a=\sqrt{\chi^2_{\theta,\phi,k_\parallel}+\frac{2m^*m_0\omega}{\hbar}}-\chi_{\theta,\phi,k_\parallel},$$
$$q_{e^\pm}=\chi_{\theta,\phi,k_\parallel}\pm\sqrt{\chi^2_{\theta,\phi,k_\parallel}-\frac{2m^*m_0\omega}{\hbar}},$$

and $\chi_{\theta,\phi,k_\parallel}=k_\parallel\sin\theta\sin\phi+(\pi/d)\cos\theta$. For scattering accompanied by phonon absorption, $\sigma_1\equiv1$. If the electron transition leads to the emission of a phonon,

$$\sigma_1=\begin{cases}0 & \text{for } \chi_{\theta,\phi,k_\parallel}<\sqrt{2m^*m_0\omega/\hbar},\\ 1 & \text{otherwise.}\end{cases} \tag{19}$$

III. RESULTS AND DISCUSSION

Figures 1 and 2 depict the results obtained for bulk GaN, a free-standing GaN QW, and an AlN/GaN/AlN QW with $d=50$ Å. In order to (a) show the details near the threshold energies and (b) keep, for the sake of simplicity, the interacting electrons in the lowest subband (QW), only a relatively small energy interval in the vicinity of Γ point is presented. Note that at higher energies all the scattering rates decrease in accordance with the general results of perturbation theory. As follows from Fig. 1, bulk scattering depends weakly on the angle between the initial electron wave vector and the c axis. This dependence is the most pronounced for the emission of phonons and manifests itself primarily for electrons with energy of the order of 0.1–0.2 eV which corresponds to the threshold values of phonon emission. Thus, this result indicates the influence of the initial configuration on the magnitude of $d(1/\tau)/dE_k$; in particular, upon increasing of electron energy, the scattering rate increases most rapidly for electron momentum oriented at $\theta_k\approx\pi/4$ for emission of TO-like phonons, and $\theta_k\approx0$ for emission of LO-like phonons. Quantization of the electron subsystem in a QW leads to the reduction of the scattering rate for all initial electron energies except for the narrow interval around $E_k\approx0.1$ eV where emission of LO-like phonons begins. The

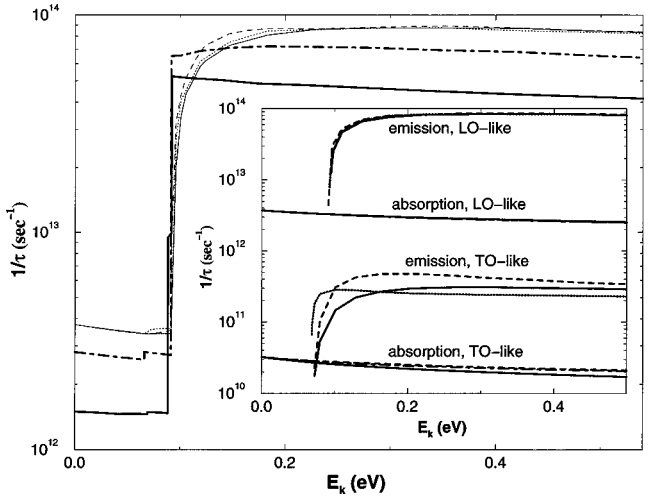

FIG. 1. Total scattering rate as a function of the electron energy, E_k. Thin lines depict scattering in the bulk system when the angle θ_k is $\pi/2$ (solid line), $\pi/4$ (dotted line), and 0 (dashed line). Confined electron-bulk phonon scattering is represented by dash-dotted line. Thick solid line depicts scattering in a GaN free-standing QW for the case when dimensionally induced transformations of spectra of both electron and phonon subsystems are taken into account. The inset shows the angle dependence of $1/\tau(E_k)$ computed for absorption and emission of TO-like and LO-like phonons in bulk GaN. The angle θ_k is $\pi/2$ (solid line), $\pi/4$ (dotted line), and 0 (dashed line).

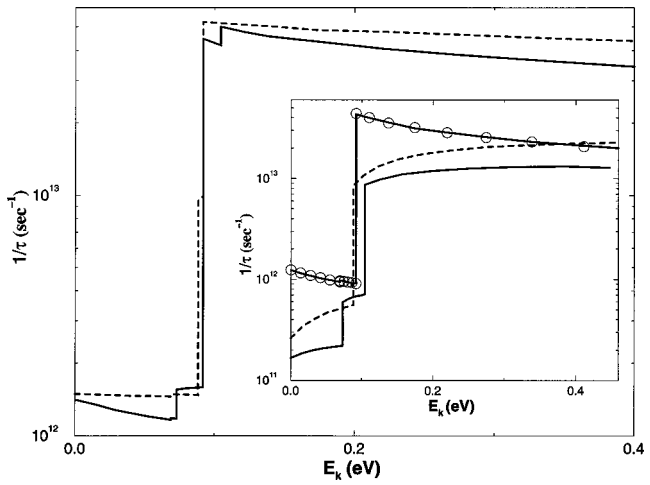

FIG. 2. Total scattering rate as a function of the electron energy E_k in GaN free-standing QW (dashed line) and AlN/GaN/AlN QW (solid line). In the inset, the upper solid line (circles) represents partial scattering on confined modes, the lower solid line (dashed line) represents partial scattering on IF modes in AlN/GaN QW (GaN free-standing QW).

sharply increasing value of $1/\tau$ for the latter case appears as a result of reduced symmetry in such a system that, eventually, induces the dependence of the wave vector of the interacting phonon subsystem on the phonon frequency provided by the requirements of energy and momentum conservation. The effect of spatial confinement of the phonon modes on the scattering of the electrons localized in the same quantum structure can be estimated by taking into account that for a free-standing QW the expression for $D(q,\omega)(^{C}_{IF})$ reduces to

$$D(q,\omega)(^{C}_{IF}) = \pi^4 \Bigg[\alpha q^2 d^2 [\pi^2 \mp (\alpha q d)^2]^2 \times \Bigg\{ [(1 \pm \xi_1^2) dq\alpha + \xi_1] 2\alpha^2 \frac{\partial \epsilon_{1z}}{\partial \omega} + [(\xi_1^2 \pm 1) dq\alpha \mp \xi_1] \frac{1}{2} \frac{\partial \epsilon_{1t}}{\partial \omega} \Bigg\} \Bigg]^{-1}. \quad (20)$$

As follows from Fig. 1, transformation of the phonon spectrum in a two-dimensional heterostructure leads to an additional decrease in the transition frequency. This size effect is as strong as the size effect of electron confinement. Moreover, the confinement of the wurtzite phonon modes in a free-standing QW results in the appearance of two phonon energy intervals allocated for confined modes and an energy interval allocated for IF modes;[10] therefore, an additional steplike feature appears in the $1/\tau(E_k)$ dependence as a result of IF phonon emission. This peculiarity leads to a slight expansion of the energy interval that corresponds to the higher scattering rate in a confined system as compared with the bulk case. In the binary-binary system, however, this enhancement disappears. As shown in Fig. 2, IF phonon emission starts at lower electron energies for AlN/GaN QW's and has a smaller magnitude. This occurs as a result of the splitting of the IF modes in such a heterostructure, where two symmetric IF modes can exist in two relatively narrow and separated intervals of phonon frequencies which correspond to TO-like and LO-like IF modes. In this case, emitted phonons are characterized by energies which are lower and higher than those of the IF phonons emitted from the free-standing QW. As expected, the emission of LO-like phonons causes a new steplike feature in the dependence $1/\tau(E_k)$.

A comparison of the scattering rates calculated for the free-standing and embedded QW's reveals another interesting feature. From the inset to Fig. 2, one can see that in both cases the energy-dependent scattering rate caused by confined phonon modes remains unchanged. At the same time, besides the additional steplike feature induced by the energy splitting, a monotonous part of $1/\tau(E_k)$ calculated for the case of scattering via IF phonons has a positive derivative in the electron energy interval which essentially exceeds the value of characteristic phonon energies. The magnitudes of these derivatives are different and, accordingly, lead to different slopes of the monotonous parts of the total scattering. Similar behavior is not unexpected for the scattering curves for confined modes. In both free-standing and embedded systems, confined TO-like and LO-like modes are located in the same energy intervals. On the other hand, the localization of electron wave function is still strong due to the relatively high potential barrier in the AlN/GaN QW. In addition, the symmetric confined modes are also well localized for almost all phonon energies as follows from the analysis of the degree of phonon confinement in such a system.[10] However, this is not true for the antisymmetric confined modes with $n=0$ and it is not true for symmetric modes in a case when the barrier material is chosen such that $\mu=1$.

The difference observed for scattering via IF phonons can be explained qualitatively as follows: IF modes in GaN free-standing QW manifest much stronger dispersion than each of

two IF modes, IF_I and IF_{II}, in an AlN/GaN heterostructure. The frequency intervals (in meV) allocated for symmetric IF modes in these systems are [69.7–95.8] for the IF modes in a free-standing GaN QW, [69.7–73.2] for IF_I, and [104.1–110.9] for IF_{II} modes. Conservation laws for a carrier which experiences intraband scattering lead to a decrease in the wave number of the absorbed (emitted) phonon as the electron energy increases. For modes with different dispersion, however, the same deviation in q would correspond to different change in ω. Since this variation is an important characteristic of the dispersive medium, one should expect that the shape of the curve $1/\tau(E_k)$ will reflect the particular dynamics of the $\omega(q)$ dependence. On the other hand, as follows from Eq. (10), the matrix element of electron-phonon interaction depends on the differences between the frequency of a phonon and characteristic frequencies rather than on absolute values of ω. As illustrated in the inset to Fig. 2, this can result in stronger scattering by IF modes in the free-standing QW even though all IF phonons in this system have lower frequencies than the IF phonons of the IF_{II} band in the embedded QW. In fact, the dependence $\omega(q)$ must not be ignored either in the matrix element or in the δ function which reflects the energy conservation law. Taking account of this additional factor results in the difference, $V_{ph}-V_{gr}$, being introduced into the denominator of the integrand in Eq. (13). At $q\sim 0.5/d$ in a GaN free-standing QW, for instance, the value of V_{gr}^{IF} becomes of the order of V_{ph}^{IF} which significantly affects the scattering of high-energy carriers. An additional consequence of the explicit account for energy conservation in the evaluation of scattering rate is the factor involving phase and group velocities that appeared from the derivative $d\theta/d\omega$. In general, the resulting transition frequency has a complex dependence on the relation between the velocities of transition of the phonon phase and energy. As illustrated by Fig. 3, even for the case when the dispersion is relatively weak, this relation may influence strongly the resulting scattering rate. Thus, our results suggest that in an optically anisotropic medium, dispersion of the phonon modes is the crucial factor that determines electron–optical-phonon scattering.

Finally, it should be emphasized that in an AlN/GaN QW it is sufficient to take into account only the two scattering mechanisms mentioned above. The propagating modes do not exist in such a system since there is no overlap in characteristic phonon frequencies. At the same time, the magnitude of the Fröhlich potential of the half-space modes would be small inside the QW.

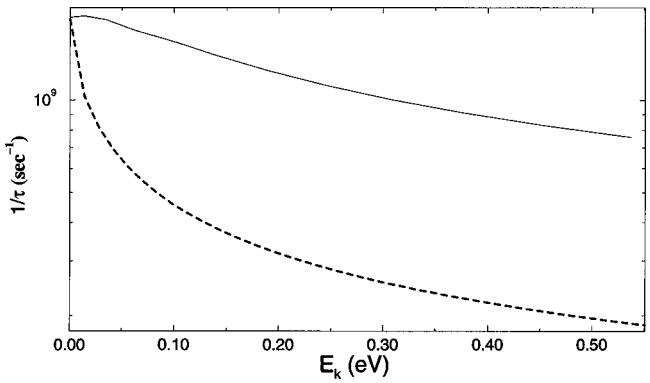

FIG. 3. Scattering rate in GaN free-standing QW via absorption of TO-like confined phonons (with relatively weak dispersion) computed for the cases when the dispersion relation is take into account (a) in matrix element only (dashed line, assuming that all absorbed phonons have energy $\hbar\omega_t$) and (b) in both matrix element and energy δ-function (solid line).

IV. SUMMARY

We have developed a formalism for the evaluation of the energy-dependent electron scattering rate resulting from interactions with infrared and Raman-active polar-optical phonons in bulk wurtzites and wurtzite-based QW's by taking into account peculiarities of the phonon spectra in uniaxial semiconductors. Our results demonstrate that the initial orientation of the carrier wave vector in a bulk crystal can determine the speed of switching of the phonon emission with respect to the electron energy, $d(1/\tau)/dE_k$. Transformation of the phonon spectra induced by reduction of the space symmetry in QW's leads to a decrease in the total transition frequency compared to the transition frequencies in bulk material and of a system of bulk phonons and confined electrons. In GaN-based heterostructures this size effect is found to be as strong as the size effect of localization of the electron wave function. Our results suggest that in optically anisotropic media, phonon dispersion affects crucially the scattering of the carriers by a particular phonon mode. This effect occurs as a result of the influence of phonon dispersion on the scattering cross section not only through the matrix element of electron-phonon interaction, but also through the selection of the appropriate momentum of the scatterer under the requirements of energy conservation.

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