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Optical phonons in GaN/AlN quantum dots: leaky modes

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Abstract

Surface polar vibrations of a GaN quantum dot in AlN matrix are analyzed in the framework of the macroscopic dielectric continuum model. The conditions are found for existence of surface modes on a quantum dot of oblate spheroidal form. These conditions determine continuum frequency regions rather than quantized frequencies. The found modes are peculiar leaky states. They can provide effective energy relaxation of the confined electrons. © 2002 Elsevier Science B.V. All rights reserved.

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Wide-band-gap nitride semiconductor materials are of substantial current interest, in view of their potential applications. The lower symmetry of their wurtzite crystal structure, compared to zinc-blende structure of conventional materials, opens the way for many new physical phenomena in electronic and phonon fields. In particular, it was found [1] that the uniaxial anisotropy of the materials involved makes confined and interface polar optical phonons in GaN/AlN quantum well quite different from those of GaAs/AlAs structure [2]. Here, we use the same macroscopic dielectric continuum model (see review in Ref. [3]) to consider surface polar vibrations of a GaN quantum dot in AlN matrix.

Retardation effects disregarded, the phonon-borne polarization in GaN ($i = 1$) and AlN ($i = 2$) is determined by the equation for the electric potential, $\psi^{(i)}(\omega, \mathbf{r})$:

$$\operatorname{div}((\hat{\varepsilon}^{(i)}(\omega)\,\mathbf{grad}\,\psi^{(i)}(\omega,\mathbf{r})) = 0 \tag{1}$$

and the boundary conditions,

$$\psi^{(1)}(\omega,\mathbf{r}) = \psi^{(2)}(\omega,\mathbf{r}), \tag{2}$$

$$(\mathbf{n}(\mathbf{r})\cdot(\hat{\varepsilon}^{(1)}(\omega)\,\mathbf{grad}\,\psi^{(1)}(\omega,r))) = (\mathbf{n}(\mathbf{r})\cdot(\hat{\varepsilon}^{(2)}(\omega)\,\mathbf{grad}\,\psi^{(2)}(\omega,r))), \tag{3}$$

where $\mathbf{n}(\mathbf{r})$ is the unit normal vector to the interface at the point $\mathbf{r}$. The frequency-dependent dielectric permittivity tensor is diagonal in the Cartesian coordinate system whose z-axis coincides with the crystallographic c-axis. Its components are

$$\varepsilon_x^{(i)} = \varepsilon_y^{(i)} = \varepsilon_l^{(i)}(\omega) = \varepsilon_\infty^{(i)}\frac{\omega^2-(\omega_{Ll}^{(i)})^2}{\omega^2-(\omega_{Tl}^{(i)})^2},$$

$$\varepsilon_z^{(i)} = \varepsilon_\tau^{(i)}(\omega) = \varepsilon_\infty^{(i)}\frac{\omega^2-(\omega_{L\tau}^{(i)})^2}{\omega^2-(\omega_{T\tau}^{(i)})^2}, \tag{4}$$

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where we assume that the high-frequency dielectric susceptibilities, ε_∞, are isotropic in both media. The values of ε_∞, along with the eight characteristic frequencies normalized to ω_{Tl} (GaAs), are given in Table 1.

Since in anisotropic media the spherical shape has no advantages of simplicity, we model the quantum dot as an oblate spheroid with the rotational axis directed along the crystallographic c-axis of AlN and GaN. Accordingly, we switch to the oblate spheroidal coordinates, u, v, and φ, so that $x = a\cosh u \sin v \cos\varphi$, $y = a\cosh u \times \sin v \sin\varphi$, $x = a\sinh u \cos v$. The surfaces $u =$ const are oblate spheroids; the dot surface corresponds to a certain $u = u_0$. The transformation of the dielectric permittivity tensor to these curvilinear coordinates produces a non-diagonal tensor:

$$\hat{\varepsilon}^{(i)}(\omega,u,v) = \begin{pmatrix} \varepsilon_1^{(i)}(\omega,u,v) & \varepsilon_2^{(i)}(\omega,u,v) & 0 \\ \varepsilon_2^{(i)}(\omega,u,v) & \varepsilon_1^{(i)}(\omega,u,v) & 0 \\ 0 & 0 & \varepsilon_\tau^{(i)}(\omega) \end{pmatrix}, \tag{5}$$

where

$$\varepsilon_1^{(i)}(\omega,u,v) = \frac{\varepsilon_\tau^{(i)}(\omega)\sinh^2 u \sin^2 v + \varepsilon_l^{(i)}(\omega)\cosh^2 u \cos^2 v}{\sinh^2 u + \cos^2 v}, \tag{6}$$

$$\varepsilon_2^{(i)}(\omega,u,v) = \frac{(\varepsilon_\tau^{(i)}(\omega) - \varepsilon_l^{(i)}(\omega))\sinh u \cosh u \sin v \cos v}{\sinh^2 u + \cos^2 v}. \tag{7}$$

Note that the off-diagonal elements $\varepsilon_2 \sim (\varepsilon_\tau^{(i)} - \varepsilon_l^{(i)})$ and thus owe their existence to the anisotropy of the media. The non-diagonality of the permittivity tensor prevents separability of the variables in Eq. (1) and the boundary conditions. This means that the solution cannot be found in general form. We restrict ourselves to considering only interface vibrations well localized near the dot surface.

Table 1

	ε_∞	$\omega_{L\tau}$	ω_{Ll}	$\omega_{T\tau}$	ω_{Tl}
GaN	5.29	1.39	1.38	1.05	1
AlN	4.68	1.72	1.68	1.26	1.24

To obtain the interface modes, we present the electric potential inside the dot, ψ_1, and outside the dot, ψ_2, in the approximate close-to-surface form,

$$\psi^{(i)}(\omega,u,v,\phi) = \exp[im\phi]\exp[\kappa^{(i)}(\omega,u_0,v)(u-u_0)] \times \chi(\omega,u_0,v), \tag{8}$$

where the inverse localization lengths, $\kappa^{(1)}$, $\kappa^{(2)} \gg 1$. Under this assumption, the localization parameters $\kappa^{(1)}$ and $\kappa^{(2)}$ and the surface part of the wave function, $\chi(\omega,u_0,v)$, are found analytically as

$$\kappa^{(i)} = \frac{|m|}{|f_0|f_1^{(i)}}\left((-1)^k f_2^{(i)}\sqrt{\frac{\varepsilon_\tau^{(1)}f_1^{(1)} - \varepsilon_\tau^{(2)}f_1^{(2)}}{F^{(1)} - F^{(2)}}} + (-1)^n\sqrt{\frac{\varepsilon_\tau^{(2)}f_1^{(2)}F^{(1)} - \varepsilon_\tau^{(1)}f_1^{(1)}F^{(2)}}{F^{(1)} - F^{(2)}}}\right), \tag{9}$$

$$\chi(\omega,u_0,v) = \text{const} \times \exp\left[-(-1)^k|m|\int\frac{dv}{|f_0|}\sqrt{\frac{\varepsilon_\tau^{(1)}f_1^{(1)} - \varepsilon_\tau^{(2)}f_1^{(2)}}{F^{(1)} - F^{(2)}}}\right], \tag{10}$$

where the auxiliary functions are

$$f_0(\omega,u_0,v) = \frac{\cosh u_0 \sin v}{\sinh^2 u_0 + \cos^2 v}, \tag{11}$$

$$f_1^{(i)}(\omega,u,v) = (\sinh^2 u + \cos^2 v)\varepsilon_1^{(i)}(\omega,u,v), \tag{12}$$

$$f_2^{(i)}(\omega,u,v) = (\sinh^2 u + \cos^2 v)\varepsilon_2^{(i)}(\omega,u,v), \tag{13}$$

$$F^{(i)} = (f_1^{(i)})^2 - (f_2^{(i)})^2. \tag{14}$$

Various choices of the integer numbers k and n in formulas (9) and (10) give four independent formal solutions. Note that the pseudo-WKB form of the surface wave function $\chi(\omega,u_0,v)$ in (10) results from the above-mentioned assumption and requires, at least, non-zero value of the angular quantum number m.

Depending on the parameters involved, not all of the obtained four independent solutions are always feasible. Specifically, to describe interface states, the obtained localization parameters, $\kappa^{(1)}$ and $\kappa^{(2)}$, should provide evanescent dependence of

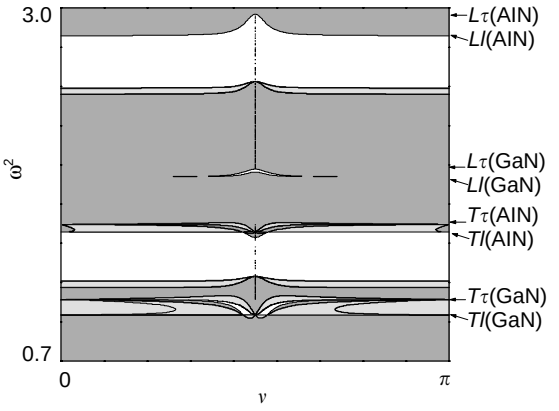

Fig. 1. Polar vibrations chart: white areas are the windows of spatial oscillations, gray areas correspond to exponential behavior, and dark areas are the escape regions.

ψ_1 and ψ_2 on $|u—u_0|$. This requirement leads to the condition

$$\mathrm{Re}(\kappa^{(1)}(u_0, v, \omega))\mathrm{Re}(\kappa^{(1)}(u_0, v, \omega)) < 0. \quad (15)$$

Given u_0, the condition (15) determines the allowed windows for the interface states in the (ω, v) plane. Within these windows, further restrictions relate to the sign of the expression under the radical in formula (10). Negative sign of this expression corresponds to spatial oscillations; positive sign corresponds to evanescent or growing exponentials. Now, the integral in formula (10) diverges logarithmically when $v \to 0$. This circumstance stipulates n to be even in the case of positive argument of the radical. In the case of negative argument of the radical, the mentioned divergence makes the surface wave function to rapidly oscillate ($\sim \sin(\ln v)$) when v approaches 0. This, in turn, means unphysical divergence of the atomic displacements at $v = 0$. Note, however, that the mentioned oscillations are essentially short-wavelength and thus cannot be treated within the model employed. Thus, we cannot completely rule out the possibility of the oscillatory states' existence.

A typical (ω^2, v) chart is presented in Fig. 1 (the squares of the bulk phonon frequencies are indicated on the right for comparison). It corresponds to moderately small value $u_0 = 0.1$. The white areas correspond to would-be spatial oscillations, the dark areas correspond to surface-state non-existence (phonon escape), and the gray areas correspond to exponential solutions. The allowed surface phonon modes fall into three categories:

(i) quasistationary, or leaky, modes, for which the regions of exponential behavior are surrounded by regions of the surface state non-existence (i.e. escape routes); the modes have their maxima at the dot poles;
(ii) penetrating modes, corresponding to the same situation but decreasing from the border of the non-existence region to the poles;
(iii) runaway modes, for which the regions of surface state non-existence neighbor the oscillatory regions.

As seen in the figure, the escape routes for quasistationary modes lie in the equatorial region of the dot. On the contrary, the runaway modes linger to the dot in the same regions.

To conclude, we have analyzed the polar surface vibrational modes of a spheroidal GaN quantum dot in AlN matrix in the approximation of close-to-surface states and found analytically their wave functions and the conditions for the mode existence. These conditions determine three basic types of the vibrational modes: leaky modes, penetrating modes, and runaway modes. The most interesting are quasistationary (leaky) states, which are connected with the surrounding continuum but linger to the dot sufficiently long to be capable of providing effective energy relaxation of the confined electrons.

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