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Polar surface vibration strips on GaN/AlN quantum dots and their interaction with confined electrons

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Abstract

The conditions are found for the existence of polar surface vibrational modes on a spheroidal quantum dot. These conditions determine allowed windows in the frequency-surface coordinate plane. The modes found are either truly localized of leaky states. The latter can provide effective energy relaxation of the confined electrons. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The uniaxial anisotropy of the wurtzite crystal structure of nitride semiconductor compounds invokes many physical phenomena having no analogues in conventional GaAs/AlGaAs heterostructures. The authors of Ref. [1] investigated polar optical phonons in GaN/AlN quantum well in the framework of the macroscopic dielectric continuum model (see review in Ref. [2]) modified to uniaxial case. In the present paper, we use the same model to consider surface polar vibrations of a GaN quantum dot in AlN matrix. We compare the obtained modes with polar vibrations of a spherical quantum dot in GaAs/AlGaAs system [3] and show that the anisotropy considerably enhances the variety of possible polar vibrations. In contrast to a series of distinct localized modes of an isotropic GaAs dot, in the GaN dot specific leaky and runaway states emerge and can play important role in the processes of electron energy relaxation.

2. Basic equations and the system parameters

In the adopted macroscopic dielectric continuum model, the phonon frequencies and wave functions in the two media labeled by index i ($i=1$ for GaN and $i=2$ for AlN) are determined entirely by the equation for the electric potential, $\psi^{(i)}(\omega,\mathbf{r})$:

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

and the boundary conditions

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

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

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Table 1

	ε_∞	$\omega_{\mathrm{L}\tau}$	$\omega_{\mathrm{L}l}$	$\omega_{\mathrm{T}\tau}$	$\Omega_{\mathrm{T}l}$
GaN	5.29	1.39	1.38	1.05	1
AlN	4.68	1.72	1.68	1.26	1.24

where $\mathbf{n}(\mathbf{r})$ is the unit normal vector to the interface at the point $\mathbf{r}$ and the frequency-dependent dielectric permittivity tensor has the form

$$\hat{\varepsilon}^{(i)} = \begin{pmatrix} \varepsilon_\tau^{(i)}(\omega) & 0 & 0 \\ 0 & \varepsilon_\tau^{(i)}(\omega) & 0 \\ 0 & 0 & \varepsilon_l^{(i)}(\omega) \end{pmatrix} \tag{4}$$

in the cartesian coordinates with the z-axis coinciding with the crystallographic c-axis

$$\varepsilon_l^{(i)}(\omega) = \varepsilon_\infty^{(i)} \frac{\omega^2 - (\omega_{\mathrm{L}l}^{(i)})^2}{\omega^2 - (\omega_{\mathrm{T}l}^{(i)})^2},$$

$$\varepsilon_\tau^{(i)}(\omega) = \varepsilon_\infty^{(i)} \frac{\omega^2 - (\omega_{\mathrm{L}\tau}^{(i)})^2}{\omega^2 - (\omega_{\mathrm{T}\tau}^{(i)})^2}. \tag{5}$$

(The high-frequency dielectric susceptibilities, ε_∞, are assumed to be isotropic in both media.) Thus, the anisotropic dielectric properties of the two media are determined by the characteristic frequencies of the longitudinal optical phonons ($\omega_{\mathrm{L}l}, \omega_{\mathrm{L}\tau}$) and the transverse optical phonons ($\omega_{\mathrm{T}l}, \omega_{\mathrm{T}\tau}$). In what follows we use the lowest of these frequencies, that of the Tl-phonon in GaN, $\omega_{\mathrm{T}l}^{(1)}$, as the frequency unit. Thus normalized, the characteristic frequencies are given in Table 1.

We model the form of the quantum dot as an oblate spheroid with the rotational axis directed along the crystallographic c-axis (the same in AlN and GaN), and use the oblate spheroidal coordinates [4]

$$x = a\cosh u \sin v \cos\phi,$$

$$y = a\cosh u \sin v \sin\phi,$$

$$z = a\sinh u \cos v. \tag{6}$$

Here, the surfaces $u = \text{const}$ are oblate spheroids; the dot surface corresponds to u_0. Transforming the dielectric permittivity tensor of Eq. (4) to these curvilinear coordinates, we obtain a non-diagonal tensor. Its off-diagonal elements emerge due to the anisotropy of the media and are proportional to $(\varepsilon_\tau^{(i)} - \varepsilon_l^{(i)})$. This non-diagonality of the permittivity tensor means that the variables in Eq. (1) (and in the boundary conditions) are no longer separable. This makes the problem of polar vibrations intractable in general form; we will only consider vibrations well localized near the dot surface.

3. Surface vibrations: formal solution

To obtain surface modes, we look for the potential inside the dot, ψ_1, and outside the dot, ψ_2, in the form

$$\psi^{(i)}(\omega, u, v, \phi) = \exp[\mathrm{im}\,\phi]\exp[\kappa^{(i)}(\omega, u_0, v)(u - u_0)]\chi(\omega, u_0, v), \tag{7}$$

where the phonon localization lengths, $\kappa^{(1)}, \kappa^{(2)} \gg 1$. Under this assumption, the wave function $\chi(\omega, u_0, v)$ and the parameters $\kappa^{(1)}$ and $\kappa^{(2)}$ obey the following system of equations:

$$\frac{\partial^2\chi}{\partial v^2} + 2\frac{f_2^{(i)}}{f_1^{(i)}}\kappa^{(i)}\frac{\partial\chi}{\partial v} + \left((\kappa^{(i)})^2 - \frac{\varepsilon_\tau^{(i)} m^2}{f_0^2 f_1^{(i)}}\right)\chi = 0, \tag{8}$$

$$f_1^{(1)}\kappa^{(1)}\chi + f_2^{(1)}\frac{\partial\chi}{\partial v} = f_1^{(2)}\kappa^{(2)}\chi + f_2^{(2)}\frac{\partial\chi}{\partial v}, \tag{9}$$

where

$$f_0(\omega, u_0, v) = \frac{\cosh u_0 \sin v}{\sinh^2 u_0 + \cos^2 v}, \tag{10}$$

$$f_1^{(i)}(\omega, u_0, v) = \varepsilon_\tau^{(i)}(\omega)\sinh^2 u_0 \sin^2 v + \varepsilon_l^{(i)}(\omega)\cosh^2 u_0 \cos^2 v, \tag{11}$$

$$f_2^{(i)}(\omega, u_0, v) = \frac{\varepsilon_\tau^{(i)}(\omega) - \varepsilon_l^{(i)}(\omega)}{4}\sinh(2u_0)\sin(2v). \tag{12}$$

The fact that the boundary condition (9) contains the v-derivative makes the solution of the system qualitatively different from the spherical harmonics obtained in Ref. [3].

We have solved system (8)–(9) analytically and obtained the following formulas for the localization lengths:

$$\kappa^{(i)} = \frac{|m|}{|f_0| f_1^{(i)}} \left(\mp f_2^{(i)} \sqrt{\frac{\varepsilon_\tau^{(1)} f_1^{(1)} - \varepsilon_\tau^{(2)} f_1^{(2)}}{F^{(1)} - F^{(2)}}} \pm \sqrt{\frac{\varepsilon_\tau^{(2)} f_1^{(2)} F^{(1)} - \varepsilon_\tau^{(1)} f_1^{(1)} F^{(2)}}{F^{(1)} - F^{(2)}}} \right), \tag{13}$$

where

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

while the wave function is found in a pseudo-WKB form

$$\chi(\omega, u_0, v) = \text{const} \times \exp\left[\pm |m| \int \frac{\mathrm{d}v}{|f_0|} \sqrt{\frac{\varepsilon_\tau^{(1)} f_1^{(1)} - \varepsilon_\tau^{(2)} f_1^{(2)}}{F^{(1)} - F^{(2)}}} \right]. \tag{15}$$

Here, the first sign in formula (13) correlates with the sign in formula (15). Thus, various choices of signs in these formulas give four independent formal solutions. This number, however, is significantly restricted by physical requirements we consider in the next section.

4. Surface vibrations: numerical analysis

To substantiate this formal solution for the surface vibration, the obtained localization parameters, $\kappa^{(1)}$ and $\kappa^{(2)}$, should satisfy the obvious condition

$$\mathrm{Re}(\kappa^{(1)})\,\mathrm{Re}(\kappa^{(2)}) < 0. \tag{16}$$

The parameters $\kappa^{(1)}$ and $\kappa^{(2)}$, being complex functions of the frequency ω and the coordinate v, condition (16) determines the allowed windows for the surface states in the (ω, v) plane. Within these windows, the character of the surface vibrations is determined by the sign of the expression under the radical in formula (15): negative sign correspond to spatial oscillations; positive sign corresponds to evanescent ("under-barrier") exponentials.

A typical (ω, v) chart (for $u_0 = 1$) is presented in Fig. 1; the areas of spatial oscillations are denoted as I, the areas of surface-state nonexistence areas (phonon escape) as II, and the under-barrier areas as III. The surface phonon modes can generally fall into three categories, marked in the figure as follows:

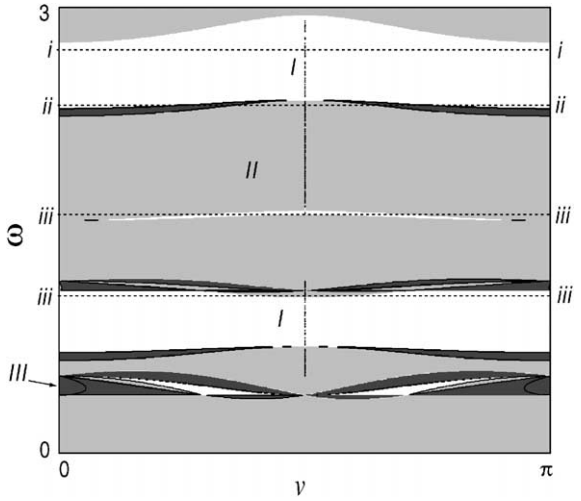

Fig. 1. Polar vibrations chart: areas of type I are the windows of spatial oscillations, areas of type III correspond to under-barrier penetration, areas of type II are the escape regions. The three possibilities for the surface states are indicated by dash lines: (i) localized states; (ii) leaky states; (iii) runaway states.

(i) truly localized modes, which sustain oscillatory character throughout the dot surface;
(ii) quasistationary, or leaky, modes; for which the regions of spatial oscillations are surrounded by barrier regions followed by regions of the surface state nonexistence (i.e. escape routes);
(iii) runaway modes, for which the regions of surface state nonexistence directly neighbor the mentioned oscillatory regions.

As seen in the figure, the escape routes for quasistationary modes and for runaway modes lie in the equatorial region of the dot. The frequencies of the surface modes and the lifetimes of quasistationary modes depend essentially on u_0, i.e. on the aspect ratio of the dot spheroid.

5. Conclusions

We have analyzed the polar surface vibrational modes of a spheroidal GaN quantum dot in AlN matrix and found analytically their wave functions and the conditions for the mode existence. These

conditions determine three basic types of the vibrational 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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