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Phonon spectrum and group velocities in wurtzite hetero-structures

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We calculated acoustic phonon spectrum and group velocities in three-layered wurtzite heterostructures. The heterostructure layer thickness has been chosen on the order of the room-temperature dominant phonon wavelength so that phonon spectrum is strongly modified compared to bulk. We derived equations of motion for different phonon polarizations in the anisotropic medium approximation, which allowed us to include the specifics of the wurtzite lattice. It has also been demonstrated that the phonon group velocity in the core layer can be made higher or lower than that in the corresponding bulk material by a proper selection of the cladding material and its thickness. Obtained results add to the concept of phonon engineering by demonstrating a possibility of enhancement of phonon transport, i.e., thermal conduction, along certain direction in heterostructures with properly tuned parameters.

1 Introduction

Heterostructures based on wurtzite materials (such as A1N/GaN/A1N and related) have been recently proposed for a variety of electronic, optical and spintronic applications. Knowledge of confined phonon spectrum in hetero- and nanostructures is important for modeling the electron transport in such structures. Recently, it was also shown that the change in the acoustic phonon spectrum induced by size quantization in hetero- and nanostructures led to significant modification of thermal transport [1,2]. In this work we present derivation of the acoustic phonon spectrum and calculation of the phonon group velocities in ultra-thin layer of wurtzite GaN embedded within A1N cladding layers. The core layer thickness d has been chosen on the order of the room-temperature dominant phonon wavelength λ so that phonon spectrum in the structure is strongly modified compared to bulk. We derived equations of motion for different phonon polarizations in the anisotropic medium approximation, which allowed us to include specifics of the wurtzite lattice. We also show that the phonon group velocity in the core layer can be made higher or lower than in the corresponding bulk material by a proper selection of the "acoustically harder" cladding material and adjusting its thickness [3, 4].

2 Theoretical approach

In order to investigate the role of the cladding material on acoustic phonon spectrum of ultra-thin films we consider a free-standing single thin film, e.g. slab, and a free-standing three-layered structure. The axis X_1 and axis X_2 are in the plane of the layers while the axis X_3 is directed perpendicular to the layer surfaces. As an example wurtzite system we first consider AlN/GaN/AlGaN heterostructure. It is further

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assumed that the layers have hexagonal symmetry with a crystallographic axis *c* directed along a coordinate axis X_3. The equation of motion for elastic vibrations in an anisotropic medium can be written as

$$\rho \frac{\partial^2 U_m}{\partial t^2} = \frac{\partial \sigma_{mi}}{\partial x_i}, \tag{1}$$

where $\vec{U}(U_1, U_2, U_3)$ is the displacement vector, ρ is the mass density of the material, σ_{mi} is the elastic stress tensor given by $\sigma_{mi} = c_{mikj} U_{kj}$, and U_{kj} is the strain tensor. When taking derivatives in Eq. (1), one has to take into account that the system is non-uniform along the X_3 axis. The elastic modules are the piece-wise functions of x_3:

$$c_{mikj} = c_{mikj}(x_3) \tag{2}$$

To reduce the number of subscript indexes in the coefficients c_{mikj}, we adopt the two-index notations. In crystals with hexagonal symmetry the following equalities are valid:

$$c_{1313} = c_{2323} = c_{44}; \; c_{1212} = c_{66} \neq c_{44}. \tag{3}$$

An application of the anisotropic continuum model allows us to explicitly include the specifics of the wurtzite crystals. The equations of motion obtained in anisotropic medium approximation with such selection of the elastic constants will be completely different from the equations of motion in the isotropic elastic medium approximation or anisotropic medium approximation for cubic crystals. The axis X_1 is assumed to be along the propagation direction of the acoustic waves. Since the three-layered structure is homogeneous in the plane (X_1, X_2), we look for the solution of the Eq. (1) in the following form

$$U_i(x_1, x_3, t) = u_i(x_3) e^{\mathbf{i}(\omega t - k x_1)} \; (i = 1, 2, 3), \tag{4}$$

where u_i are the amplitudes of the displacement vector components, ω is the phonon frequency k is the phonon wave vector and $\mathbf{i}$ is imaginary unity. A shear polarization, e.g. the displacement vector is parallel to the structure surfaces, can be distinguished from the others using the following definition

$$\rho \frac{\partial^2 U_2}{\partial t^2} = \frac{\partial \sigma_{2i}}{\partial x_i}. \tag{5}$$

By substituting Eq. (4) for *i=2* to Eq. (5) and taking into account Eqs. (2-3), one can turn the partial differential Eq. (5) into an ordinary second order differential equation

$$-\rho\omega^2 u_2(x_3) = c_{44} \frac{d^2 u_2(x_3)}{dx_3^2} + \frac{dc_{44}}{dx_3} \cdot \frac{du_2(x_3)}{dx_3} - c_{66} k^2 u_2(x_3). \tag{6}$$

Derivatives $\frac{dc_{ik}}{dx_3}$ account for the fact that the structure is heterogeneous. In the case of a slab, one can obtain a simple analytical solution from Eq. (6) by setting $\frac{dc_{44}}{dx_3} = 0$. The external surfaces of the three-layered structure are assumed to be free. As a result, the force components along all coordinate axes

equal to zero, e.g., $P_1 = P_2 = P_3 = 0$, where $P_i = \sigma_{ik} n_k$, and $\vec{n}$ is the vector normal to the surfaces of the structure. Thus, on the outer surfaces of the structure the following relationship is satisfied

$$\frac{\partial u_2}{\partial x_3} = 0; \tag{7}$$

For the two other vibrational polarizations (*i*=1,3) with the displacement vector components U_1 and $U_3^{'} = -\mathbf{i} U_3$ we obtain from Eqs. (1) and 94) the following system of two interrelated equations

$$-\rho\omega^2 u_1(x_3) = -k^2 c_{11} u_1(x_3) + c_{44} \frac{d^2 u_1(x_3)}{dx_3^2} + k(c_{13} + c_{44}) \frac{du_3^{'}(x_3)}{dx_3} + \frac{dc_{44}}{dx_3}\left(\frac{du_1(x_3)}{dx_3} + k u_3^{'}(x_3)\right), \tag{8}$$

$$-\rho\omega^2 u_3^{'}(x_3) = -k^2 c_{44} u_3^{'}(x_3) + c_{33} \frac{d^2 u_3^{'}(x_3)}{dx_3^2} + \frac{dc_{33}}{dx_3} \frac{du_3^{'}(x_3)}{dx_3} - k\left[(c_{44} + c_{13}) \frac{du_1(x_3)}{dx_3} + \frac{dc_{13}}{dx_3} u_1(x_3)\right], \tag{9}$$

with the following boundary conditions on the outer surfaces of the structure

$$\frac{du_1}{dx_3} + k u_3^{'} = 0, \quad -k c_{13} u_1 + c_{33} \frac{du_3^{'}}{dx_3} = 0. \tag{10}$$

Due to the spatial symmetry of the considered three-layered structure and the mathematical form of Eqs. (8-9), the displacement vector should have components with an opposite parity, e.g., (u_1^S, u_3^A) or (u_1^A, u_3^S), where $u_i^S(x_3)(i = 1,3)$ is a symmetrical function of x_3 while $u_i^A(x_3)$ (*i*=1, 3) is an anti-symmetrical function of x_3. We will denote the symmetric (SA) and anti-symmetric (AS) displacement vectors with the corresponding upper indices. Thus, the displacement vectors $\vec{u}^{SA} = \vec{u}(u_1^S, u_3^A)$ and $\vec{u}^{AS} = \vec{u}(u_1^A, u_3^S)$ define independent polarizations, which, together with the shear modes, compose a full set of normal vibrational modes in the structure. In the case of a slab the SA modes are referred to as dilatational modes while AS modes are termed the flexural modes.

3 Results and discussion

To obtain the phonon dispersion, we solve the differential Eq. (6) with boundary condition of Eq. (7) for shear polarization, and the system of Eqs. (8) and (9) subject to the boundary conditions of Eq. (10) for SA and AS polarizations. The equations are solved using the finite difference method [3, 4]. The calculations are performed for each value of the phonon wave vector *k* from the interval $k \in (0, \pi/a)$, where *a* is the lattice constant in the plane (X_1, X_2). After obtaining the phonon dispersion, we calculate the phonon group velocity as a function of *k*. In Fig. 1 we show the dispersion relation $\hbar\omega_n^{sh}(k)$ and the group velocity $v_n^{sh}(k)$ for a set of shear modes. Figure 1(a) presents data for a GaN slab with thickness d=6 nm. Figure 1(b) presents data for the AlN/GaN/AlN heterostructure. One can see from Fig. 1 that in the zone center, the phonon group velocity is a liner function of the phonon wave vector $v_n^{sh}(k) = a_n k$. With increasing *k* all phonon dispersion curves approach a limit $\hbar\omega_0(k) = v_0 \hbar k,$ where $v_0 = v^{TA_2}(GaN)$ is the velocity of the transverse acoustic wave propagating along X_1 axis and polarized along X_2 axis. For very large values of *k*, all phonon modes in the slab become GaN bulk-like. Strong size- quantization of the phonon spectrum for small values of *k* leading to the emergence of the quasi-

optical modes and significant decrease of the phonon group velocity ($v_n(k) < v^{TA_2}(GaN)$) constitute the phonon confinement effects in an ultra-thin slab. These effects were shown to have a pronounce influence on the lattice (phonon) thermal conductivity of semiconductor quantum wells, when calculated with actual full phonon spectrum [1].

The inhomogeneity of the three-layered structure changes the shape of the dispersion curves both quantitatively and qualitatively. For large *n* at large *k* the phonon modes are (AlN, TA_2) bulk–type. The phonon modes in the multi-layered structure are formed as result of superposition of vibrations from different layers on the structure interfaces, which leads to the mode hybridization. Depending on the *k* value the hybrid modes can reveal signatures of the specific layers signatures rather then those of the averaged structure properties. For example, the group velocity for the mode with *n=1* at moderate *k* is $v^{TA_2}(AlN)$, while at large *k* the group velocity is $v^{TA_2}(GaN)$ despite the fact that the total width of the cladding AlN layers is five times larger than the width of the core GaN layer. The group velocity of the mode with $n = 5$ tends monotonically to the bulk velocity $v^{TA_2}(AlN)$.

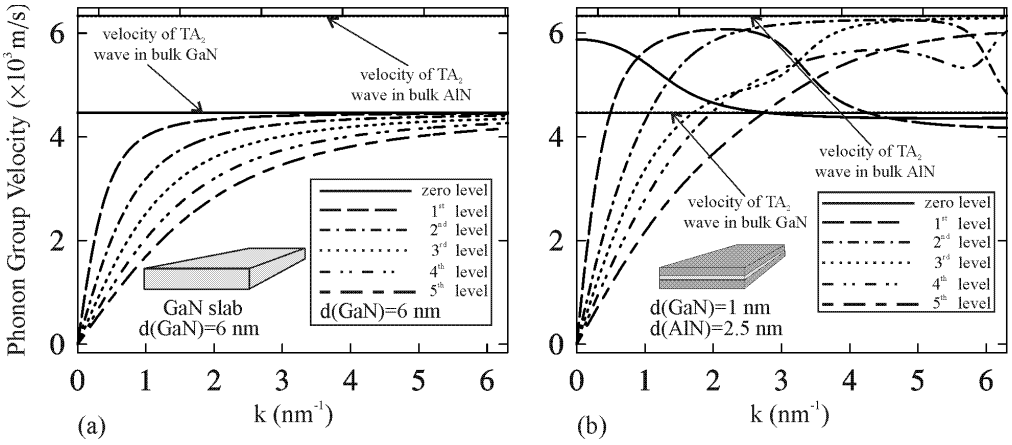

Fig. 1 Phonon group velocities as functions of the phonon wavevector for the shear polarization. Results are shown for (a) 6 nm wide slab and (b) three-layered heterostructures with dimensions 2.5 nm / 1 nm/ 2.5 nm. In the figure legend, the level is defined by the quantum number *n* unlike the phonon mode, which is defined by the quantum number and wave vector *k*.

Overall in the ultra-thin slabs, the phonon group velocity decreases due to the phonon confinement effect [1], while in the three-layered heterostructure with "acoustically hard" cladding layers, the phonon group velocity can be larger than the bulk phonon velocity in the core layer material. One should note here, that the results are obtained for the coherent phonon transport regime ($d \sim \lambda$), when the phonon waves extend though the whole structure and "feel" the presence of the boundaries. A possibility of tuning the phonon group velocity may have a profound effect on thermal transport in hetero- and nanostructures [1-3] as well as on carrier-phonon scattering rates [4–6].

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