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Vibrational modes and symmetry in a hexagonal cross-section nanowire

六角形断面を持つナノワイヤーの対称性と振動モード

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1. Introduction

Recently, various nanowire structures have been synthesized. The properties of the wires are often superiour to the bulk's ones, which lead to their applications in many areas. In particular, nanowires of III-V semiconductor (GaN, AlN, and InN) are attractive because of their direct bandgaps (0.7 eV in InN to 6.2 in AlN), which are desirable for optoelectronic applications. Nanowire superlattices (NWSLs) constructed from these III-V semiconductors are also attractive for use in semiconductor devices because strain accomodation allows the combination of materials with large acoustic mismatch without dislocations.

To improve electronic devices (e.g. their high electron mobility and high thermal conductivity), understanding the acoustic phonons in the nanowire is of imporatnce. In addition, these structures yield interesting physical effects on phonon properties.

The NWSLs can be regarded as wire-type phononic crystals (PhCs). The remarkable behavior of the PhCs are related to the appearance of phononic bandgaps [1-3]. In the NWSLs, the phononic band gaps are induced by the periodicity along the wire axis. The PhC can be regarded as an barrier for the phonons winthin the phononic bandgaps [4, 5]. This leads to designing various phonon optics devices, such as phonon filters, mirrors, resonators and so on [6].

In a previous paper [7], we theoretically studied the acoustic phonon modes in GaN/AlN NWSLs, and determined a set of parameters which gives complete phononic bandgaps. In the paper [7], circular cross-section NWSLs with a zinc-blende structure were considered. Most of thin III-V nanowires have a wurtzite structure and their cross-sections are hexagonals. In general, phonon modes in a NWSL depend on the shape of the cross-section of the wire. Thus, we need to study the influence of the cross-section shape on the vibrational modes.

In the present proceedings, as a first step, we theoretically examine acoustic phonon modes in a hexagonal cross-section GaN nanowire with a wurtzite structure. In addition, we consider a hollow GaN nanowire, and examine the effect of the thickness of this nanotube on the dispersion relations.

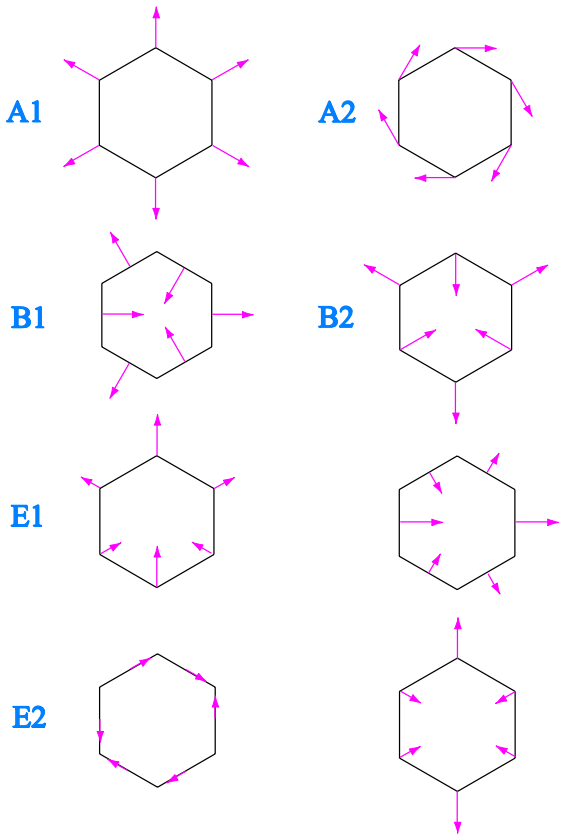

Fig. 1. Symmetry-adopted basis functions belonging to the irreducible representations of C_{6v}. Arrows show the phonon displacements at the high-symmetry points.

2. Method

The method we used is the XYZ algorithm [8]. The equation giving the eigenfrequencies of phonon modes in a freestanding NWSL composed of anisotropic crystals was given in Ref. [9]. In the

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present study, we derive the analytical expressions for the matrix elements we need. By using the symmetry-adopted basis functions, the dispersion relations and phonon displacements are obtained for each phonon mode.

3. Symmetry and vibrational modes

The group of k is C_{6v} for $0 < |k| < \pi / D$. The irreducible representations are A_1, A_2, B_1, B_2, E_1, and E_2. Using their projection operators, we can construct symmetry-adopted basis functions belonging to the irreducible representations of this group [10]. The symmetries of the basis functions are schematically shown in **Fig. 1**. In this figure, the phonon displacements at the high-symmetry points are shown. The A_1 , A_2 , and E_1 modes correspond to dilatational, torsional, and flexural modes, respectively.)

4. Numerical results and discussions

Figure 2(a) shows the phonon dispersion relations calculated for the solid GaN nanowire. Here, k is the Bloch wave number in the longitudinal direction. Subband structure exists in the dispersion relation. This is due to the fact that the wave vectors in the lateral direction are discretized because of the lateral confinement of phonons.

The lowest eight curves correspond to the E_1, A_2, A_1, E_1 and E_2 modes, as shown in Fig. 2(a). All the dispersion curves of the E_1 and E_2 modes are doubly degenerated. The dispersion curves of B_1 and B_2 modes exist in higher frequency range.

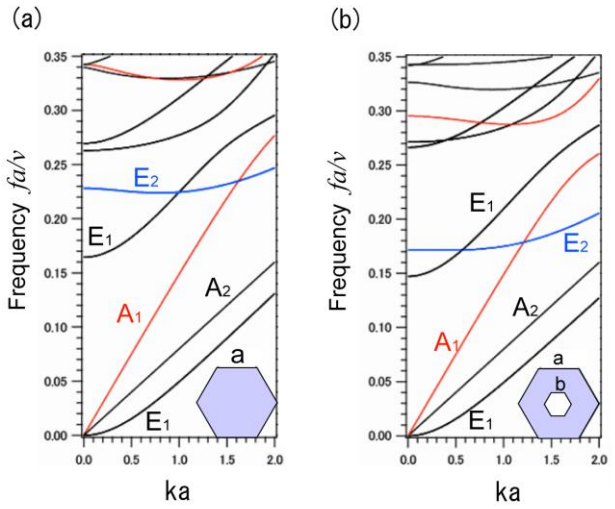

Fig. 2 Phonon dispersion relations of the haxagonal cross-section NWSL consisting of wurtzite GaN: (a) solid and (b) hollow wires (a/b = 4). The dispersion curves of the E_1 and E_2 modes are doubly degenerated.

The lowest dispersion curves of the A_1 and A_2 modes are linear in k (i.e., the frequencies vanish at $k = 0$). On the other hand, the lowest frequencies of the B_1 , B_2 and E_2 modes have finite values. For thin (thick) NWSLs, the lowest frequencies of B_1 , B_2 and E_2 modes become higher (lower). For the E_1 modes, the lowest dispersion curve near $k = 0$ is proportional to k^2. This is due to the fact that these modes correspond to bending.

Figure 2(b) shows the dispersion relations for the hollow GaN nanowire. Compared with Fig.2(b), the dispersion curve of the E_2 mode shifts largely to the lower frequency range. In thinner nanowires, the dicretized wavelengths in the lateral directions become shorter. As a result, subbands except for lower subbands of the A_1, A_2 and E_1 modes go up to the higher frequency range. However, in the hollow nanowires, the subbands of the E_2 modes exist in the lower frequency range.

4. Conclusions

In the present paper, we theoretically studied the acoustic phonon modes in a hexagonal cross-section GaN nanowire. We calculated their dispersion relations. The acoustic phonon modes are classified into 6 types, i.e., A_1, A_2, B_1, B_2, E_1 and E_2 modes. We found that only the eigen-frequencies of the E_2 modes is sensitive to the ratio of inner side and outer side of the hexagonal hollow nanowire. The results for the GaN/AlN nanowire superlattice will be given elsewhere.

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