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Phonon Dispersion Relations of GaN/AlN Nanowire Superlattices with Circular Cross-sections

円形断面を持つ GaN/AlN ナノワイヤー超格子のフォノン分散関係

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1. Introduction

Phononic crystals (PCs) are composite materials made of arrays of constituents embedded in host materials [1-3]. The interesting behavior of these PCs is related to the existence of frequency gaps (i.e., phononic band gaps) due to the Bragg reflections of the phonons with long wavelengths. We can regard the PC as an opaque barrier for these phonons [4, 5]. This suggests the potential for designing various phonon optics devices, such as phonon filters, mirrors, resonators and so on [6].

Recent advances in fabrication methods enable realization of one-dimentional hetero-structures, i.e., nanowire superlattices (NWSLs) [7-10]. Their electronic and optical properties were studied, and a variety of possible applications utilizing the characteristics were also proposed. In addition, the NWSLs are expected to yield interesting physical effects on phonon properties. The NWSL can be regarded as a wire-type phononic crystal (WPC), in which the phononic band gaps are induced by the periodicity along the wire axis.

In a previous paper [11], we developped a numerical method to derive all phonon modes in a free-standing NWSL of anisotropic material with an arbitrary shape of cross-section. In this paper, as examples, the phonon modes were calculated for the rectangular and square cross-section GaAs/AlAs NWSLs composed of anisotropic materials. Though this result revealed the important aspects of phonon modes in the NWSLs, it seems to be difficult to design WPCs with complete phononic band gaps because in the dispersion relations of the GaAs/AlAs NWSL many subbands are folded into the mini-Brillouin zone and the frequencies of gaps are different with phonon modes. In addition, the widths of the frequency gaps are narrow in this NWSL because the difference of the acoustic impedance between the GaAs and AlAs layers is small. To realize the phonon optics devices (e.g., filters, mirrors, and resonators), the NWSLs with large acoustic mismatch, such as GaN/AlN NWSLs, would be suitable.

In the present work, we calculate numerically the dispersion relations and corresponding displacement fields for a NWSL consisting of GaN and AlN, and we determine a set of parameters which gives complete frequency gaps.

2. Method

The equation giving the eigenfrequencies of phonon modes in a freestanding NWSL composed of anisotropic crystals was formulated in Ref. [11].

The phonon modes can be classified with the use of group theory [12, 13]. In the present study, constituent layers are assumed to consist of cubic materials. The group of k is C_{4v} for $0<|k|<\pi/D$. The irreducible representations of C_{4v} are A_1, A_2, B_1, B_2, E, which have features of dilatational, torsional, stretching, shear, and flexural modes, respectively [11].

By considering the above symmetry, the symmetry-adapted basis function in the present system can be constructed, and the phonon dispersion relations of each mode are independently calculated.

3. Numerical results and discussions

Semiconductor NWSLs from group III-V and group IV materials have been synthesized with the use of nanocluster catalysts [7-10]. The shapes of the cross-sections of these NWSLs are considered to be the circles whose radii are determined by the diameters of the nanocluster catalysts. The typical dimensions have been nanowire radii (R) of 10-50 nm and layer widths (D) of 1-100 nm. In the present example, we selected that R = 5.0 nm and D = 25.0 nm so that the complete gaps are generated.

Other parameters we used are as follows: ρ = 6.15 g/cm³, C_{11} = 2.96, C_{12} = 1.54, and C_{44} = 2.06 (all in units of 10^{12} dyn/cm²) for GaN; ρ = 3.26 g/cm³, C_{11} = 3.04, C_{12} = 1.52, and C_{44} = 1.99 (all in units of 10^{12} dyn/cm²) for AlN [14].

Figure 1 shows the calculated phonon dispersion relations. In the present frequency range,

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we can see three different modes, i.e., A_1, A_2, and E modes. The dispersion curves corresponding to B_1 and B_2 modes exist in higher frequency range.

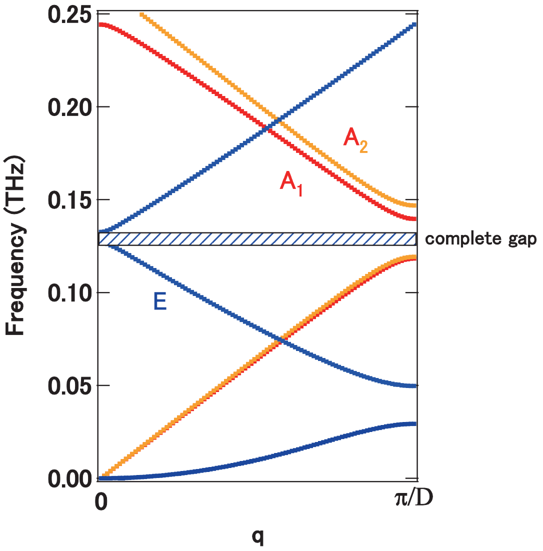

Fig. 1 Phonon dispersion relations of the circular cross-section NWSL consisting of GaN and AlN with R=5nm and D=25 nm. For GaN and AlN layers, cubic lattice are assumed.

These dispersion relations can be explained with the effects of both the confinement of phonons in the lateral direction and superlattice modulation in the longitudinal direction. The overall structure of each phonon dispersion relation can be approximately understood by the folding of the dispersion curves for a homogeneous plain nanowire into a mini-Brillouin zone determined by the periodicity D of the NWSL. In an isolated wire, the boundary condition at the free surface of the wire requires that the wave numbers in the lateral direction are discretized. On the other hand, the wave number k in the longitudinal direction has a continuous value. Therefore, the dispersion relation of the homogeneous plain nanowire has subband structure.

In thinner nanowires, the dicretized wavelengths in the lateral directions become shorter. As a result, subbands except for lower subbands of A_1, A_2 and E modes go up to the higher frequency range. On the other hand, the unit period along the wire axis of the NWSL determines the size of the mini-Brillouin zone, i.e., frequencies of the gaps are determined by the unit period D. Changing the ratio of the radius R and D, we can control the phonon modes in the lower frequency range.

In the present example, we selected R = 5.0 nm and D = 25.0 nm (thicknesses of GaN and AlN layers are 12.5 and 12.5 nm, respectively) so that the first frequency gaps of the A_1 and A_2 and the second gaps of the E_1 modes are located in the similar frequency range.

The above results suggest the realization of the design of the optimized phonon devices for phonon generation or control, such as mirrors, filters, and also resonators. These are expected to be applicable to the micro/nano electromechanical systems.

4. Conclusions

We found that the complete frequency gap can be realized for GaN/AlN NWSLs. In the present paper, we only showed the results for GaN/AlN nanowire superlattices consisting of “cubic” GaN and AlN. The results for those of “hexagonal” GaN and AlN will be given elsewhere.

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