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Variational method with Legendre-basis-functions: calculation of acoustic phonon modes in nanowires

対称性を考慮したルジャンドル関数を用いた変分法によるナノワイヤーの振動モード計算

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1. Introduction

During the last decade, various kinds of nanowires (NWs) have been synthesized. The properties of the NWs are often superiour to the bulk's ones, which lead to their applications in many areas. Very recently, a lot of NWs with complicated structures such as nanowire superlattices (NWSLs) and radial nanowire heterostructures have been realized [1, 2]. To improve electronic devices, e.g. their high electron mobility and high thermal conductivity, understanding acoustic phonons in the NWs is of imporatnce. In addition, these structures yield interesting physical effects on phonon properties.

Acoustic phonons in these structures are expected to show reduced-dimensional behaviour depending on thier geometry. In general, it is difficult to obtain acoustic phonon modes in such wire structures due to the longitudinal acoustic (LA) and transverese acoustic (TA) wave coupling occuring at the wire surface or interfaces of the nanowires. For example, even in rectangular cross section isotropic NWs, the LA and TA phonons coupling makes it difficult to derive phonon modes and their spectra analytically.

A numerical method for deriving the free vibrational modes of anisotropic object with arbitrary shape was developped in the resonant ultrasound spectroscopy [3]. In this method, the displacement vectors are expanded in terms of a set of basis functions. Since products of x, y, and z are used as basis functions, this scheme is called xyz algorithm. This method was shown to be appricable for free-standing plain nanowires [4] and nanowire superlattices [5]. For the NWs with complicated sturucture, on the other hand, a lot of basis functions are needed to express the lattice displacement vectors.

To carry out an accurate calculation, in the present study, we use the Legendre functions as basis functions instead of the powers of the Cartesian coordinates.

As numerical examples, we examine acoustic phonon modes in a hollow GaN NW and a hollow GaN/AlN NWSL with a circular cross-section. We compare the calculated eigenfrequencies with those obtained by the xyz algorithm, and discuss the efficiency of this method.

In the present proceedings, we give a brief sketch of our fomulation and show the results calculated for a hollow GaN NW.

2. Method of Calculation

The displacement vectors u_i, which are solution of the elastic equation

$$\rho\omega^2 u_i + \frac{\partial}{\partial x_j}\left(C_{ijk\ell}\frac{\partial u_k}{\partial x_\ell}\right) = 0 \qquad (1)$$

with boundary conditions

$$T_{ij}n_j = 0 \qquad (2)$$

at surface, make the Lagrangian defined by

$$L[u_i] = \int_V \left[\frac{1}{2}\rho\omega^2 u_i u_i - \frac{1}{2}C_{ijk\ell}\frac{\partial u_i}{\partial x_j}\frac{\partial u_k}{\partial x_\ell}\right] dV \qquad (3)$$

stationary. In Eq. (3), we expand u_i in terms of the basis functions φ_λ,

$$u_i = \sum_{\lambda\in\Omega} a_{i\lambda}\varphi_\lambda \qquad (4)$$

Here, Ω means a truncated one of the complete set of the basis functions. The stationary condition imposed on Eq. (3) becomes $\partial L/\partial a_{i\lambda} = 0$, which gives

$$H_{\beta i,\alpha\ell}a_{\alpha\ell} = \omega^2 S_{\beta i,\alpha\ell}a_{\alpha\ell}, \qquad (5)$$

where

$$H_{\beta i,\alpha\ell} = \sum_{j,k}\int_V \frac{\partial\varphi^*_\beta(\mathbf{r})}{\partial x_j}C_{ijk\ell}(z)\frac{\partial\varphi_\alpha(\mathbf{r})}{\partial x_k}d\mathbf{r}, \qquad (6)$$

and

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$$S_{\beta i,\alpha\ell} = \delta_{i\ell}\int_V \varphi_\beta^*(\mathbf{r})\rho(z)\varphi_\alpha(\mathbf{r})dV\,. \qquad (7)$$

Solving (5), we can determine the eigenmodes in the free-standing NWs.

For simplicity, in the present proceedings, we show the basis function selected for the hollow NW with circular cross-section:

$$\varphi_\alpha(k,\mathbf{r}) = \frac{1}{\sqrt{S}} P_m\left(\frac{x}{R}\right)P_n\left(\frac{y}{R}\right)e^{ikz}\,. \qquad (8)$$

Here, k is the wave number in the longitudinal direction, P_m is the Legendre function, R denotes the radius of the wire, and S is the cross-sectional area of the hollow structure. The basis functions are specified with m,n, that is, $\alpha=(m,n)$. In the plain wire stiffness tensor $C_{ijk\ell}(z)$ and mass density $\rho(z)$ are independent of the coordinate.

Substituting (8) into (7), we have

$$S_{\beta i,\alpha\ell} = \rho\delta_{i\ell}\times \frac{1}{S}\int_S P_m\left(\frac{x}{R}\right)P_n\left(\frac{y}{R}\right)P_{m'}\left(\frac{x}{R}\right)P_{n'}\left(\frac{y}{R}\right)dS, \qquad (9)$$

where $\beta=(m',n')$. This integral depends on the geometry of the cross-section of the wire. In the complicated structures, Eq. (9) does not give the orthogonal relation. In the present study, we successfully derived the analytical expressions for this and also Eq. (6). However, we cannot show them here because these are legthy.

In general, many basis functions are needed to represent the displacement fields. By utilizing group theory and classifying the phonon modes, the number of basis functions can be reduced. The C_{2v} symmetry is included in most NWs. In this case, the modes are classified into A_1, A_2, B_1, B_2 modes. Then, only a quarter of basis functions are necessary, and the number of matrix elements we should calculate becomes one sixteenth.

By using the symmetry-adapted basis functions, the dispersion relations and phonon displacements are calculated for each phonon mode. For NWs with high symmetry, each classified mode is further classified. In the calculation, it is convenient to classify one of the above modes according to the symmetry of corresponding eigenvector calculated from Eq. (5).

3. Numerical results and discussions

We show in Fig.1 the phonon dispersion relations calculated for a hollow NW consisting of wurtzite GaN. The ratio of the inner diameter ($2r$) of the hollow circular cross section to the outer diameter ($2R$) is assumed to be 0.5 in this example.

Subband structure exists in the dispersion relation, because the wave vectors in the lateral direction are discretized. The lowest four curves correspond to the B_1, B_2, A_2, and A_1 modes, as shown in Fig. 1. The dispersion curves of the B_1 and B_2 modes are doubly degenerated in the present symmetry.

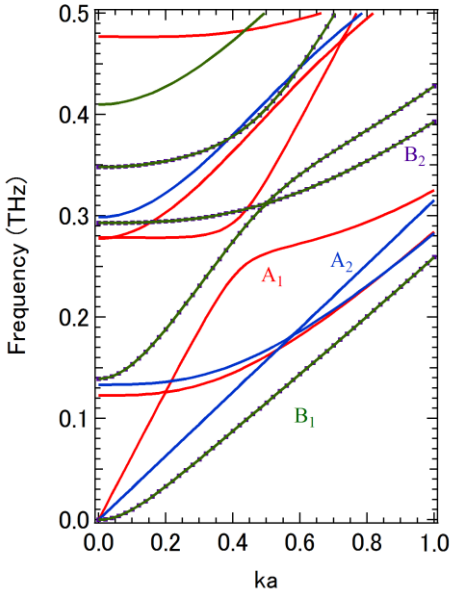

Fig. 1 Phonon dispersion relations of the hollow NW consisting of wurtzite GaN ($r/R=0.5$).

4. Concluding remarks

We have developed a variational method with symmetry-adapted Legendre basis functions. The detailed explanation and comparison with the dispersion relations obtained with different methods will be given elsewhere.

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