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# Vibrational modes in wire-type phononic crystals with square and circular cross-sections
# 正方形断面および円形断面をもつワイヤー型フォノニック結晶に生じる振動モード

Yushi Nakamura[†] and Seiji Mizuno[1] (Facult. Eng., Hokkaido Univ.)
中村祐史[‡]，水野誠司（北大 工）

## 1. Introduction

Phononic crystals (PCs) are composite materials made of one-, two-, or three-dimensional arrays of constituents embedded in host materials. The remarkable behavior of these PCs is related to the existence of phononic band gaps due to the Bragg reflections of phonons with long wavelengths.

Recently, advances in fabrication methods enable realization of one-dimensional compositionally modulated nanowires. For example, GaAs/GaP, Si/SiGe and InAs/InP, nanowire superlattices (NWSLs) were synthesized, and their electronic, optical, and transport properties were studied[1-7]. The NWSLs were shown to be offer unique features. These are radically different from plain nanowires and quantum wells in their electronic, optical, and transport properties. On the other hand, modifications in the normal modes of phonons in the NWSLs have not been well studied, though 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. Generally speaking, it is hard to derive analytically the phonon modes in theWPCs. The only exception is acoustic torsional modes in a cylindrical WPC of elastically isotropic materials. In a previous paper[8], we studied theoretically the torsional modes in a circular cross-section WPC consisting of "isotropic" materials, using the potential function method and transfer matrix method. Although this work revealed the important aspects of phonon modes in the WPC, characteristics of the other modes are not understood. Furthermore, the dispersion relations of a WPC depend on the shape of its cross-section.

Very recently, we formulated a method to derive phonon modes in a free-standing WPC of “anisotropic” material with an arbitrary shape of cross-section[9]. Using this method, in the present work, we calculate the dispersion relations and phonon displacement field for square and circular cross-section WPCs, and examine all the phonon modes in these WPCs.

## 2. Numerical results and discussions

As a numerical example, we consider in the present work square and circular cross-section WPCs consisting of the alternate stacking of InAs and InP. In the present paper, we show only the results for the square cross-section WPC.

The thickness of the wire and the unit period (D) along the wire axis are assumed to be 100 Å and 85.0 Å, respectively (InAs and InP have the same length in the z direction). Other parameters we used are as follows: $\rho = 5.68$ g/cm$^3$, $C_{11} = 83.3$, $C_{12} = 45.3$, and $C_{44} = 39.6$ (all in units of $10^{10}$ dyn/cm$^2$) for InAs; $\rho = 4.81$ g/cm$^3$, $C_{11} = 102.2$, $C_{12} = 57.6$, and $C_{44} = 46.0$ (all in units of $10^{10}$ dyn/cm$^2$) for InP, where $\rho$ and $C_{\mu\nu}$ are the mass density and stiffness tensor, respectively.

The phonon modes in the square cross-section WPC can be classified with the use of group theory. The translational symmetry along the wire axis is considered in the wave numbers $k$. While the point group of the unit cell is $D_{4h}$, the group of $k$ is $C_{4v}$ for $0 < |k| < \pi / D$.

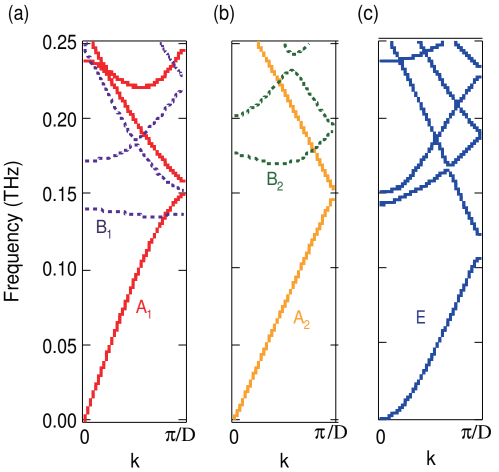

**Fig. 1** Phonon dispersion relations of the square cross-section NWSL consisting of InAs and InP. (a) $A_1$ mode (solid lines) and $B_1$ mode (dashed lines), (b) $A_2$ mode (solid lines) and $B_2$ mode (dashed lines), and (c) E modes. In (c), all dispersion curves are doubly degenerated.

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[1] Electronic address: mizuno@eng.hokudai.ac.jp

The irreducible representations of $C_{4v}$ are $A_1$, $A_2$, $B_1$, $B_2$, and E. Fig. 1 shows the phonon dispersion relations calculated for these five modes. 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 cylinder into a mini-Brillouin zone determined by the periodicity $D$ of the WPC. Subband structures exist in the dispersion relations of the homogeneous plain nanowire, because the lateral confinement of phonons discretizes their wave vectors in the lateral direction.

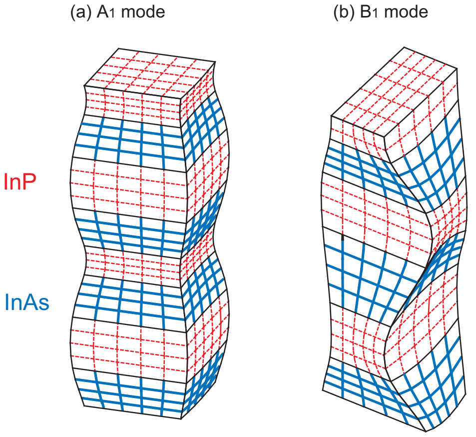

**Fig. 2.** Displacement field patterns in a square cross-section InAs/InP WPC: (a) the lowest dilatational ($A_1$) and (b) lowest stretching ($B_1$) modes at q=π/D.

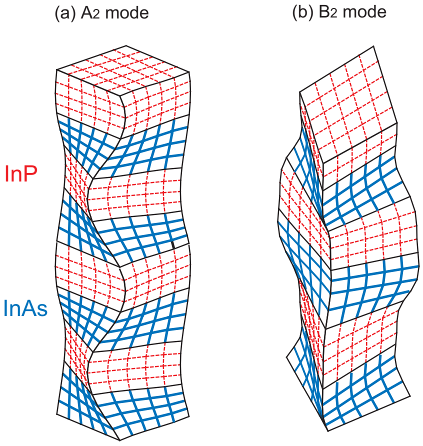

**Fig. 3.** Displacement field patterns in a square cross-section InAs/InP WPC: (a) the lowest torsional ($A_2$) and (b) lowest shear ($B_2$) modes at q=π/D.

The calculated displacement patterns corresponding to the lowest dispersion curves of the five modes at $k = \pi / D$ are illustrated in Figs. 2 to 4. These figures clearly show that the $A_1$, $A_2$, $B_1$, $B_2$, and E modes have features of dilatational, torsional, stretching, shear, and flexural modes, respectively.

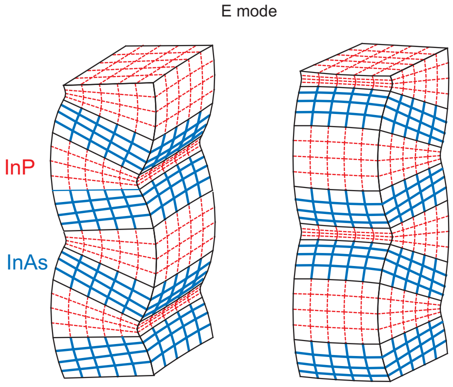

**Fig. 4.** Displacement field patterns in a square cross-section InAs/InP WPC: the lowest flexural modes (E modes) at q=π/D.

## 4. Conclusions

In the present paper, we theoretically studied the acoustic phonon modes in a square cross-section InAs/InP WPC. We calculated their dispersion relations and phonon displacement fields. The acoustic phonon modes are classified into five types, i.e., $A_1$, $A_2$, $B_1$, $B_2$, and E modes, which have features of dilatational, torsional, stretching, shear, and flexural modes, respectively.

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