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Size-effect on band structures of nanoscale phononic crystals

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ABSTRACT

The scaling law does not hold when the sizes of the phononic crystals reach the nanoscale dimension [Ramprasad et al., Applied Physics Letters 87 (2005) [9]]111101. This paper discusses the size-effect on the band structures of nanoscale phononic crystals. The transfer matrix method based on the nonlocal elastic continuum theory is developed to compute the band structures of a nanoscale layered phononic crystal. Detailed calculations are performed for a nanoscale HfO_2–ZrO_2 multilayer stack. It is shown that the nonlocal elastic continuum solution deviates from the classical elastic continuum one and finally approaches the first-principle result as the thickness of each individual layer decreases. When the thickness of each layer is much larger than several nanometers, the correspondence between the nonlocal and classical elastic methods is shown, and the size effects can be neglected. The developed nonlocal elastic continuum method is expected to overcome the limits of the classical continuum description for wave propagation in phononic crystals when dimensions are in nanometer-length scales.

1. Introduction

Phononic crystal (PNC), which was first proposed by Kushwaha et al. [1], is a kind of composites composed of periodic arrays of two or more materials with different mass densities and elastic properties. It exhibits complete band gaps in its transmission spectra, where the propagation of acoustic or elastic waves is strictly forbidden in all directions. By introducing defects (point, linear or planar) to break the periodicity of the systems, it is possible to create highly localized defect or guided modes within the acoustic band gaps. Because of these distinguishing features, PNCs seem to be one of the most promising candidates for design of new acoustic devices such as wave detectors, filters, waveguides, transducers, acoustic lenses, acoustic interferometers, etc. The last decades have witnessed great research interest, both experimental and theoretical, in PNCs [2].

With the rapid development of the technology in the fields of communication information, medical engineering, etc., the size of acoustic devices is required to be smaller and smaller. For instance, the gigahertz communication generally requires the nanosized devices. The hypersonic phononic band gaps could be used to design new thermo-electric devices, acoustic-optic devices, nanoelectric-mechanical systems (NEMS), etc. [3–5]. Recently, the manufacture, measurement and computation of the hypersonic PNC together with its application in manipulation of hypersonic acoustic waves have received considerably more and more attention [6–8].

It is known that the size-effect will become more important and should be taken into account when a system is in the dimension of several nanometers. Ramprasad and Shi [9] presented the phononic band structure calculations for a nanoscale HfO_2–ZrO_2 multilayer stack using the first-principle method at the atomistic level and by solving the classical elastic wave equation at the continuum level, and found that the results from the first-principle are quite different from those by the plane wave expansion method based on the classical elastic (CE) continuum theory. They pointed out that the scaling law [10], i.e. uniformly expanding or shrinking the physical sizes of the photonic or phononic crystals by a factor β results in the frequency spectrum being scaled by $1/\beta$, does not hold when the sizes of the PNCs reach the nanoscale dimension. This implies the size-dependence of the wave propagation behavior in a nanosized PNC. Their study indicated the need for careful treatments of wave propagation properties for PNCs at the nanometer-length scales. Hepplestone and Shrivastava [11] also highlighted the limits of the CE theory when they studied the hypersonic phonon modes in periodically arranged composite semiconductors using the ball-and-spring model.

In this paper, the band structure calculations of a nanoscale layered PNC have been implemented using the transfer matrix method based on the nonlocal elastic (NLE) continuum theory. The NLE continuum theory was established due to the early efforts of Kroener and Datta [12], Kunin [13], Green and Rivlin [14], Eringen [15] and Edelen [16] and was well summarized in

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a recent monograph by Eringen [17]. It takes into account the effects of the long range interatomic forces, which become more pronounced when the structure size is comparable with the atomic constant. It explains successfully the dispersion phenomenon of plane waves with very high frequency propagating in a homogeneous elastic medium discovered in phonon dispersion experiments [17]. Recently, the NLE theory has been used to study mechanical behaviors of nanoscale structures where the size-effects must be taken into account [18–36].

2. Nonlocal elastic theory

Unlike the CE theory, which assumes that the stress at a point is solely dependent on the local strain field at this point, the NLE theory takes into account the effects of the long range interatomic forces and supposes that the stress-state at a point is related to the strain-state at all points of the entire body, so that the constitutive relations are written as [17]

$$\tau_{kl}(\mathbf{x}) = \int_V \alpha(|\mathbf{x}'-\mathbf{x}|)\sigma_{kl}(\mathbf{x}')\mathrm{d}v(\mathbf{x}'), \quad k,l=1-3, \tag{1}$$

where $\mathbf{x}$ is the position vector, τ_{kl} are the nonlocal stress components and σ_{kl} are the stress components calculated by the CE theory, which, for the homogeneous and isotropic medium, are given by

$$\sigma_{kl}(\mathbf{x}') = \lambda e_{rr}(\mathbf{x}')\delta_{kl} + 2\mu e_{kl}(\mathbf{x}'), \tag{2}$$

with

$$e_{kl}(\mathbf{x}') = \frac{1}{2}\left(\frac{\partial u_k(\mathbf{x}')}{\partial x_l'} + \frac{\partial u_l(\mathbf{x}')}{\partial x_k'}\right), \tag{3}$$

where λ and μ are Lamé constants, and u_k are the displacement components. In Eq. (1), $\alpha(|\mathbf{x}'-\mathbf{x}|)$ is the influence function, which is dependent on the internal characteristic length ε (e.g. the atomic lattice constant). It acquires its maximum at $\mathbf{x}'=\mathbf{x}$, attenuating with $|\mathbf{x}'-\mathbf{x}|$. When $\varepsilon\to 0$, $\alpha(|\mathbf{x}'-\mathbf{x}|)$ reduces to the Dirac delta function $\delta(|\mathbf{x}'-\mathbf{x}|)$, and then Eq. (1) reverts to the constitutive equations of CE theory. On the other hand, when ε approaches the external characteristic length (e.g. the wavelength, the structure size, etc.), the NLE theory should approximate discrete theories (e.g. the atomic lattice dynamics, etc.). The influence function $\alpha(|\mathbf{x}'-\mathbf{x}|)$ for a particular material can be determined by matching the dispersive curves obtained from the NLE theory with those from the first-principle theory, atomic lattice dynamics or experiments. More detailed properties of $\alpha(|\mathbf{x}'-\mathbf{x}|)$ and determination of its particular form may be found in Ref. [17]. Here for the one-dimensional problem considered in this paper, we will choose the following simple form [17]:

$$\alpha(|x|,\varepsilon) = \frac{1}{2\varepsilon}\mathrm{e}^{-(|x|/\varepsilon)}. \tag{4}$$

The constitutive equation of the integral form, Eq. (1), can be approximated by a differential one [17]:

$$(1-\varepsilon^2\nabla^2)\tau_{kl} = \sigma_{kl}, \tag{5}$$

where ∇^2 is the Laplace operator. The dynamic equilibrium equations without body forces are

$$\tau_{kl,l} = \rho\ddot{u}_l, \tag{6}$$

with ρ being the mass density. Substitution of Eqs. (2), (3) and (5) in Eq. (6) yields the following differential wave motion equation of the NLE theory:

$$(\lambda+\mu)u_{k,lk} + \mu u_{l,kk} = (1-\varepsilon^2\nabla^2)\rho\ddot{u}_l. \tag{7}$$

3. Problem statements and band structure calculation

A layered PNC consisting of layers (sub-cells) A with thickness d_1 and B with thickness d_2 alternatively as shown in Fig. 1 will be studied in this paper; d_1 and d_2 are at the nanoscale. Consider a harmonic elastic wave propagating normally in the system. The term $\mathrm{e}^{-\mathrm{i}\omega t}$ where $\mathrm{i}=\sqrt{-1}$ and ω is the frequency will be suppressed throughout this paper without misunderstanding. Then by introducing the dimensionless local coordinate $\xi_j = x_j/d$, where $d=d_1+d_2$ and $0\le\xi_j\le\bar{d}_j \triangleq d_j/d$ with $j=1$ and 2 representing the sub-cells A and B, respectively, Eq.(7) can be reduced to the following simple form for the present one-dimensional problem:

$$\frac{\partial^2 u_j}{\partial\xi_j^2} + \frac{u_j}{\varpi_j^{-2}-R_j^2} = 0, \tag{8}$$

where $R_j=\varepsilon_j/d$ is the ratio of the internal to external characteristic lengths, $\varpi_j=\omega d/c_j$ are the non-dimensional frequencies and the wave velocity $c_j = c_{Lj} = \sqrt{(\lambda_j+2\mu_j)/\rho_j}$ for the longitudinal wave and $c_j = c_{Tj} = \sqrt{\mu_j/\rho_j}$ for the transverse wave.

From Eq. (8) one can obtain the dispersion equation for the one-dimensional wave in the bulk materials A and B:

$$k_j^2 = \frac{1}{(c_j/\omega_j)^2-\varepsilon_j^2}, \tag{9}$$

where k_j is the bulk wave number in material A ($j=1$) or B ($j=2$). The internal characteristic length ε_j, which may vary for different materials, can be determined by matching the dispersion curves obtained from Eq. (9) with those from the first-principle theory, atomic lattice dynamics, experiments, etc.

The general solution of Eq. (8) can be obtained as

$$u_j(\xi_j) = A_{1j}\mathrm{e}^{-\mathrm{i}q_j\xi_j} + A_{2j}\mathrm{e}^{\mathrm{i}q_j\xi_j}, \tag{10}$$

where $q_j = \sqrt{\varpi_j^2/(1-R_j^2\varpi_j^2)}$.

From Eqs. (1)–(3) and Eq. (10), we can obtain the stress component

$$\begin{aligned}\tau_j(\xi_j) &= \frac{\rho_j c_j^2}{2R_j}\int_0^{\bar{d}j}\mathrm{e}^{-|\xi_j-\zeta|/R_j}\frac{\partial u_j(\zeta)}{\partial\zeta}d\zeta \\ &= \frac{-\mathrm{i}\rho_j c_j^2 q_j}{2}\left(\frac{\mathrm{e}^{-\mathrm{i}q_j\xi_j}-\mathrm{e}^{-\xi_j/R_j}}{1-\mathrm{i}R_jq_j} - \frac{\mathrm{e}^{-\mathrm{i}q_j\bar{d}_j}\mathrm{e}^{-(\bar{d}_j-\xi_j)/R_j}-\mathrm{e}^{-\mathrm{i}q_j\xi_j}}{1+\mathrm{i}R_jq_j}\right)A_{1j} \\ &\quad + \frac{\mathrm{i}\rho_j c_j^2 q_j}{2}\left(\frac{\mathrm{e}^{\mathrm{i}q_j\xi_j}-\mathrm{e}^{-\xi_j/R_j}}{1+\mathrm{i}R_jq_j} - \frac{\mathrm{e}^{\mathrm{i}q_j\bar{d}_j}\mathrm{e}^{-(\bar{d}_j-\xi_j)/R_j}-\mathrm{e}^{\mathrm{i}q_j\xi j}}{1-\mathrm{i}R_jq_j}\right)A_{2j}.\end{aligned} \tag{11}$$

Next the band structures for the present layered PNC will be calculated by following a procedure that is similar to the transfer matrix method for the CE theory [37]. Take $\mathbf{V}=\{u,\tau\}^{\mathrm{T}}$ as the state

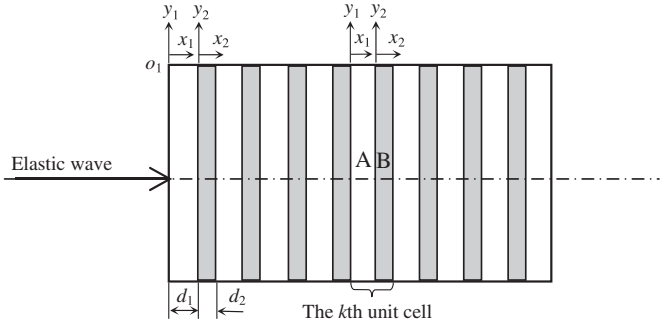

Fig. 1. Schematic diagram of a one-dimensional layered phononic crystal.