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Bandgap calculation of in-plane waves in nanoscale phononic crystals taking account of surface/interface effects

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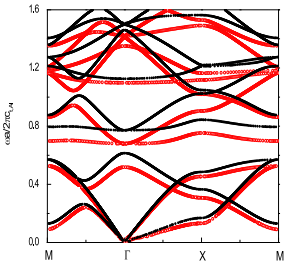
HIGHLIGHTS

- The DtN-map method is extended to research the in-plane waves in nanoscale PNCs.
- We generalize a surface parameter to characterize the surface/interface effects.
- The surface/interface effects have significant influences on the band structures.

GRAPHICAL ABSTRACT

The band structures of the PNC of a square lattice of vacuum cylindrical holes in aluminum matrix without (black) and with (red) the surface effect.



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ABSTRACT

In the present paper, the band structures of in-plane waves propagating in two-dimensional nanoscale phononic crystals composed of voids/inclusions in an elastic solid in square and triangular lattices are calculated by the method based on the Dirichlet-to-Neumann map. The surface/interface effects are taken into account due to the high surface-to-volume ratio by applying the Young–Laplace equilibrium equation at the surface/interface. Three systems at nanoscale are calculated in details: vacuum holes in an aluminum matrix in square and triangular lattices, aluminum cylinders in tungsten matrix in a square lattice, and tungsten cylinders in aluminum in a square lattice. The results show that the surface/interface effects are significant when the dimensions of the phononic crystals approach the nanometer scale.

1. Introduction

In recent years, acoustic devices toward to miniaturization and components of those in micro/nanometer length scale, such as micro- and nanoelectromechanical systems (i.e. MEMS and NEMS), etc., received considerable attention due to the rapid development of the information technology. When the mechanical functionality of the advanced materials is investigated, the significant influence of the surface/interface energy and stresses which resulted from the high surface-to-volume ratio cannot be neglected [1–3], and most properties of the nanoscale materials and structures have been demonstrated to be size-dependent [4]. In this case, the classical elastic continuum theory cannot predict the mechanical behaviors of the systems correctly. Thus the surface/interface effects must be taken into account. To this end, Gurtin et al. [5,6] established a theory of surface elasticity, according to which the surface/interface is regarded as a negligibly thin membrane adhered to the abutting bulks without slipping. To date, the theory of surface elasticity has been widely used to evaluate the effects of size-dependent phenomena for nanocomposites [7–9]. Here we particularly mention the studies in the field of wave propagation. Wang et al. [10,11] devoted their investigations to the

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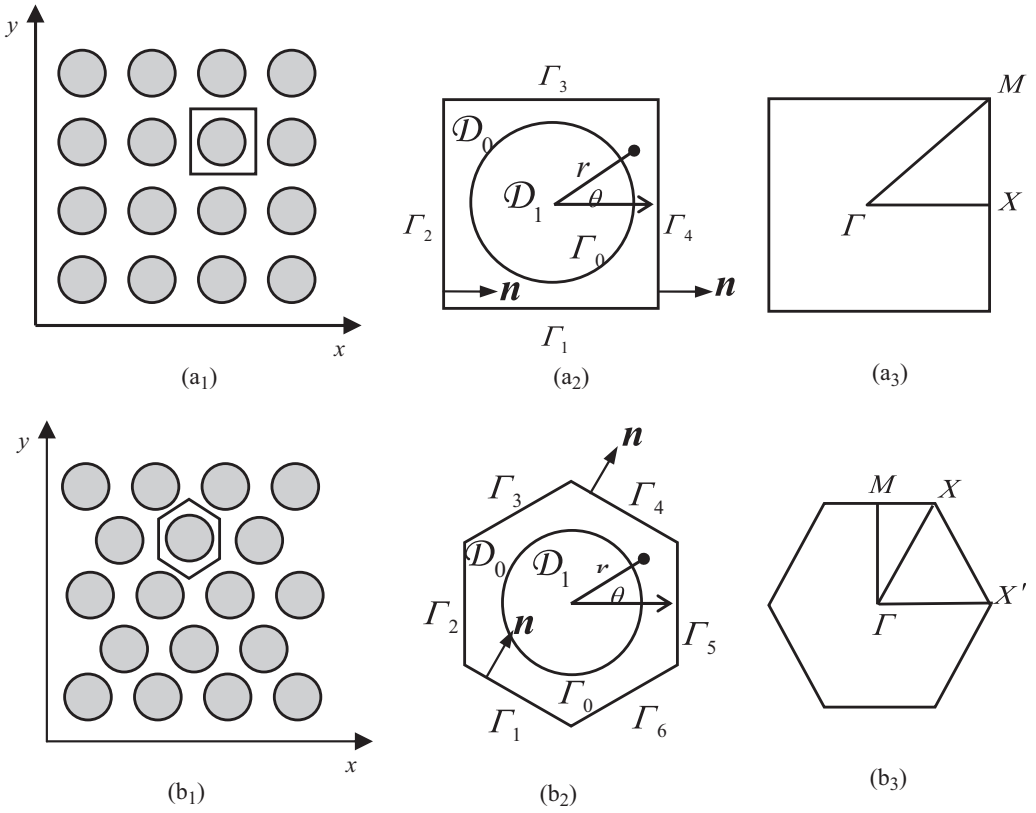

Fig. 1. The square lattice (a_1) with the unit cell (a_2) and the corresponding first Brillouin zone (a_3); and the triangular lattice (b_1) with the unit cell (b_2) and the corresponding first Brillouin zone (b_3).

research on the diffraction of elastic waves in nanostructures considering the surface/interface effects. Hasheminejad and Avazmohammadi [4] indicated that the interface elasticity at nanometer length scales can significantly alter the overall dynamic mechanical properties of nanofiber-reinforced composites.

In the past decades, phononic crystals (PNCs) [12] which are a kind of artificial periodic structures have been drawing considerable attention worldwide. The distinguishing feature of PNCs is the existence of the bandgaps where the elastic waves cannot propagate through the structures. PNCs have potential applications in acoustic filters, noise suppression, vibration isolation and design of new acoustic devices [13,14]. Recently the fabrication and analysis of phononic crystals at nanoscale, the so-called hypersonic phononic crystals [15–19], have been demonstrated. This provides a new way to explore the applications in acousto-optic modulation, electron–phonon engineering, heat management, etc. [20–25]. It has been indicated that the particular treatments of wave propagation properties for nanoscale PNCs are necessary when the elastic continuum theory is applied. Chen and Wang [26] developed a transfer matrix method based on the nonlocal elastic continuum theory to calculate the band structures of a nanoscale HfO_2–ZrO_2 multilayer stack. Their results revealed that the nonlocal elastic continuum solution deviated from the classical elastic continuum one, i.e. the band structures of nanoscale PNCs are size-dependent. Other researchers also showed that the theory of surface elasticity might be another candidate to overcome the limits of the classical elastic continuum theory. For instance, based on the interface model developed by Gurtin and Murdoch [6], Zhen et al. [27,28] extended the method of Dirichlet-to-Neumann (DtN) map [29–31] to investigate the transverse waves propagating in two-dimensional (2D) nanoscale PNCs composed of circular holes or inclusions and discussed the surface/interface effects in details; Liu et al. [32] used the multiple scattering theory (MST) [33–35] to calculate the band structures of 2D PNCs composed of nanoscale holes in a square lattice.

In the present paper, we will extend the DtN-map method [36] to explore the mixed in-plane wave modes propagating in two-dimensional nanoscale phononic crystals taking into account the surface/interface effects. Both hole/solid and solid/solid systems in square and triangular lattices will be considered. The dependence of the upper and lower edges of the first bandgap on the surface moduli and the filling fraction will be analyzed. We will introduce and generalize a surface parameter characterizing the surface/interface effects, and discuss the influence of this parameter which may positive or negative, on the band structures.

2. Problem formulation

At the nanoscale, we consider a 2D phononic crystal composed of circular holes or elastic solid inclusions with radius r_0 in an isotropic elastic solid matrix in a square or triangular lattice with the lattice constant a. Fig. 1 shows the lattice structures, the unit cells and the corresponding first Brillouin zones. Γ_1–Γ_4 (or Γ_1–Γ_6) represent the external edges of the square (or hexagonal) unit cell; Γ_0 denotes the surface of the hole or interface between the matrix and the inclusion. The Cartesian coordinates (x,y) and the polar coordinates (r,θ) on the xy-plane are related by $\mathbf{x}=(x,y)=(r\cos\theta, r\sin\theta)$, with the origins of the coordinates located at the center of the unit cell.

We consider harmonic mixed in-plane elastic waves propagating in the xy-plane. Therefore all wave field quantities such as the displacements, stresses, strains, etc. are harmonic functions of time. The harmonic wave equations can be written as [37]

$$(\lambda_j+\mu_j)\nabla(\nabla\mathbf{u}_j)+\mu_j\nabla^2\mathbf{u}_j+\rho_j\omega^2\mathbf{u}_j=0,\quad j=0,1 \tag{1}$$