A METHOD FOR CALCULATING THE ELASTIC WAVE BAND STRUCTURE OF TWO-DIMENSIONAL PHONONIC CRYSTALS WITH INTERFACE/SURFACE STRESS EFFECT

Wei Liu[*], Xianyue Su[*a)]
[*]*LTCS and Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing, 100871, China*

Summary In the present work, based on the interface/surface elasticity, the authors extend the multiple scattering theory method for calculating the elastic wave band structure of two dimensional phononic crystals (PCs) with interface/surface stress effect at the nanoscale. Elastic Mie scattering matrix embodying the interface/surface stress effect is derived. Numerical results manifest the significant effect of interface/surface stress on the elastic wave band structure of two-dimensional PCs.

INTRODUCTION

Elastic wave propagation in artificial periodic composites termed as phononic crystals (PCs) has recently attracted much attention due to the underlying rich physics [1-2]. In addition, the frequency band gaps and other unusual properties, such as negative refraction, sub-wavelength imaging and localization confer PCs many attractive potential applications.

Recently, the possibility of fabricating and measuring micro and nano PCs have been demonstrated and the integration of devices based on PCs into communication and sensing systems has been anticipated in pace with the development of nanotechnologies. It has long been known that interface/surface stress may have significant effect on the mechanical and other physical behaviors of smallsized materials and structures due to the high interface/surface-to-volume ratio. Gurtin [3] and Murdoch and Gurtin et al [4] have developed the interface/surface elasticity theory to describe the interface/surface stress effect in the continuum framework, which has been demonstrated to be capable of well reproducing the results of direct atomic simulations.

To date, little attention has been paid to the interface/surface stress effect on the wave propagation in PCs, which is of practical importance for designing and characterizing miniaturized devices based on PCs. In this paper, we extend the multiple scattering theory (MST) method by incorporating the interface/surface elasticity theory and investigate the interface/surface stress effect on the elastic wave band structure of two-dimensional PCs.

MST WITH INTERFACE/SURFACE STRESS EFFECT TAKEN INTO ACCOUNT

Consider two-dimensional (2D) PCs consisting of aligned cylindrical inclusions or pores periodically embedded in a matrix. According to the MST, the elastic wave band structure of 2D PCs can be obtained by solving the following secular equation [5]

$$\det\left|\sum_{n''\zeta''} t_{n''\zeta''n'\zeta'}\, g_{n''\zeta''n\zeta}(\mathbf{k}) - \delta_{nn'}\delta_{\zeta\zeta'}\right| = 0 \tag{1}$$

where δ is the Kronecker delta, $\mathbf{k}$ is the Bloch wave vector. The index ζ, running from 1 to 3, represents three wave modes, i.e. the longitudinal mode (ζ=1) and the two shear modes (ζ=2,3). $g_{n''\zeta''n\zeta}$ is defined as

$$g_{n''\zeta''n\zeta}(\mathbf{k}) = \sum_{\mathbf{R}_N \neq \mathbf{0}} e^{i\mathbf{k}\cdot\mathbf{R}_N} G_{n''\zeta''n\zeta}(\mathbf{R}_N) \tag{2}$$

where the right-hand side is conditionally convergent and difficult to be directly evaluated with high accuracy. Alternatively, it can be calculated using the method by Chin et al [6].

For conventional PCs, the elastic Mie scattering matrix $\mathbf{T}=\{t_{n\zeta n'\zeta'}\}$, which relates the incident wave expansion coefficients $\mathbf{A}=\{a_{n\zeta}\}$ and the scattered wave expansion coefficients $\mathbf{B}=\{b_{n\zeta}\}$, can be obtained from the displacement and traction continuity conditions at the interface of the matrix and the scatterer.

However, when the interface/surface stress effect is taken into account, according to interface/surface elasticity, the traction continuity condition at the interface of the matrix and the scatterer should be replaced by

$$[\boldsymbol{\sigma}_1(\mathbf{r}) - \boldsymbol{\sigma}_2(\mathbf{r})]\cdot\mathbf{e}_r\,|_{r=a} = -\nabla_s\cdot\boldsymbol{\tau} \tag{3}$$

where $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ are the stress in the matrix and inclusion, respectively, a the radius of the scatterer. $\nabla_S\cdot\boldsymbol{\tau}$ denotes the interface/surface divergence of the interface/surface stress $\boldsymbol{\tau}$. For a linear elastically isotropic interface/surface, the relation between the interface/surface stress $\boldsymbol{\tau}$ and the interface/surface strain $\boldsymbol{\varepsilon}^s$ is of the following form

$$\boldsymbol{\tau} = \lambda_s(\mathrm{tr}\,\boldsymbol{\varepsilon}^s)\mathbf{I} + 2\mu_s\boldsymbol{\varepsilon}^s \tag{4}$$

where λ_s and μ_s are the interface/surface elastic moduli. Eq. (3) as well as the displacement continuity condition

$$[\mathbf{u}_1(\mathbf{r}) - \mathbf{u}_2(\mathbf{r})]\,|_{r=a} = \mathbf{0} \tag{5}$$

gives rise to the following equations:

a) Corresponding author. Email: xyswsk@pku.edu.cn.

$$\begin{cases} A_{11}a_{n1} + A_{21}a_{n2} + B_{11}b_{n1} + B_{21}b_{n2} = C_{11}c_{n1} + C_{21}c_{n2} \\ A_{12}a_{n1} + A_{22}a_{n2} + B_{12}b_{n1} + B_{22}b_{n2} = C_{12}c_{n1} + C_{22}c_{n2} \\ A_{13}a_{n1} + A_{23}a_{n2} + B_{13}b_{n1} + B_{23}b_{n2} = C_{13}c_{n1} + C_{23}c_{n2} \\ A_{14}a_{n1} + A_{24}a_{n2} + B_{14}b_{n1} + B_{24}b_{n2} = C_{14}c_{n1} + C_{24}c_{n2} \\ A_1 a_{n3} + B_1 b_{n3} = C_1 c_{n3} \\ A_2 a_{n3} + B_2 b_{n3} = C_2 c_{n3} \end{cases} \tag{6}$$

Solving Eq. (6) yields the elastic Mie scattering matrix **T** embodying the interface/surface stress effect. Comparison of **T** with and without interface/surface stress effect reveals that the interface/surface stress effect is completely characterized by two additional dimensionless parameters $k_1=(\lambda_s+2\mu_s)/(\mu_1 a)$ and $k_2=\mu_s/(\mu_1 a)$, from which size-dependence of the interface/surface stress effect on the band structure of 2D PCs can be directly identified. For macroscopic PCs with large scatterer radius a, k_1 and $k_2<<1$, the interface/surface effect can be neglected and **T** reduces to that with no interface/surface stress effect. However, as the radius of the scatterer shrinks to nanometers, k_1 and k_2 would become significant and the interface/surface stress effect cannot be neglected.

NUMERICAL RESULTS AND DISCUSSIONS

Consider a 2D PC composed of aligned infinite holes embedded in an aluminum matrix and arranged in square lattice, which is sketched in Fig.1. The radius of the hole and the lattice constant are set to be 4.1nm and 10nm, respectively, resulting in a filling ratio of 0.53. The material parameters of aluminum are mass density ρ=2697 kg/m^3, Lamé constants λ=52.09 GPa and μ=34.7 GPa. Two sets of surface elastic constants [7] are employed, which are denoted as surface A (λ_s=3.489 N/m , μ_s=-6.218 N/m) and surface B (λ_s =6.842 N/m , μ_s =-0.376 N/m), respectively.

Fig. 2 depicts the elastic wave band structure of the 2D square lattice PC for in-plane modes. It is clearly evidenced in Fig. 2(a), where surface A is considered, that the surface stress effect significantly influences the band structure, and the influence is more prominent in the relatively high frequency regime. For the 2D square lattice PC with surface A, the frequency bands for in-plane modes shift downwards as the surface stress effect is considered. In addition, the first band gap becomes wider due to the surface stress effect, extending from the normalized frequency 0.6474 to 0.7760 without surface stress effect while being from 0.5839 to 0.7294 as the surface stress effect is considered. Similar effects can be observed in the band structure for out-of-plane modes and thus omitted here due to space limit.

Fig. 2(b) shows the case of surface B. Again, it is manifested that the surface stress would considerably affect the band structure. However, in contrast to those in Fig. 2(a), the frequency bands shift upwards as the surface stress effect is present. Additionally, with the surface stress being considered, the first complete band gaps becomes narrower, which is different from the case of surface A.

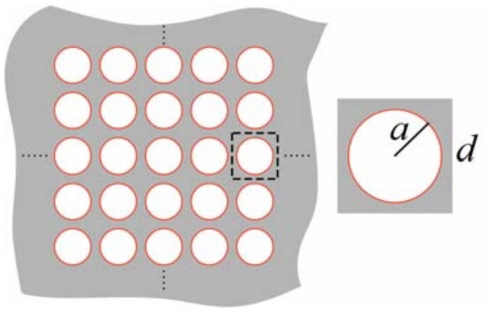

Fig. 1 Sketch of the 2D square lattice PC composed of aligned infinite holes embedded in aluminum.

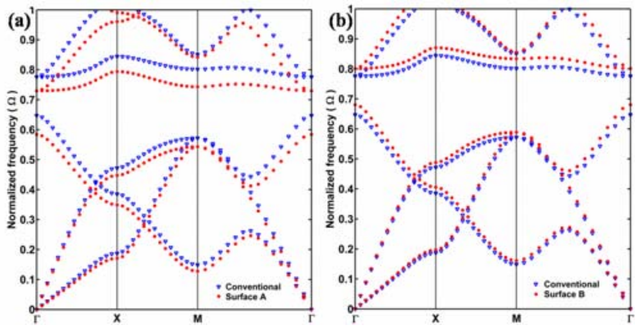

Fig. 2 Band structure of the 2D square lattice PC for in-plane modes: (a) surface A; (b) surface B.

CONCLUSIONS

In summary, the interface/surface elasticity is employed to describe the nonclassical conditions at the interface/surface and the MST is accordingly extended to investigate the interface/surface stress effect on the elastic wave band structure of 2D PCs in this paper. Numerical examples for a 2D PC show that the surface stress effect on the band structure would be significant as the characteristic size reduces to nanometers.

References

[1] Sigalas M. M., Economou E. N.: *J. Sound. Vib* **158**(2): 377-382, 1992.
[2] Kushwaha M.S., Halevi P., Dobrzynski L, Djafarirouhani B.: *Phys Rev Lett* **71**: 2022-2025, 1993.
[3] Gurtin M.E., Murdoch A.I.: *Arch Ration Mech An* **57**: 291-323, 1975.
[4] Gurtin M.E., Weissmuller J., Larche F.: *Philos Mag A* **78** : 1093-1109, 1998.
[5] Mei J., Liu Z.Y., Shi J., Tian D.C.: *Phys Rev B* **67**: 245107, 2003.
[6] Chin S.K., Nicorovici N.A., Mcphedran R.C.: *Phys Rev E* **49**: 4590-4602, 1994.
[7] Miller R.E., Shenoy V.B.: *Nanotechnology* **11**: 139-147, 2000.