Anti-plane transverse waves propagation in nanoscale periodic layered piezoelectric structures

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Abstract In this paper, anti-plane transverse wave propagation in nanoscale periodic layered piezoelectric structures is studied. The localization factor is introduced to characterize the wave propagation behavior. The transfer matrix method based on the nonlocal piezoelectricity continuum theory is used to calculate the localization factor. Additionally, the stiffness matrix method is applied to compute the wave transmission spectra. A cut-off frequency is found, beyond which the elastic waves cannot propagate through the periodic structure. The size effect or the influence of the ratio of the internal to external characteristic lengths on the cut-off frequency and the wave propagation behavior are investigated and discussed.

Keywords Nanoscale; Piezoelectricity; Localization factor; Band structure; Nonlocal piezoelectric continuum theory; Transfer matrix method; Stiffness matrix method.

1. Introduction

Orderly layered structures refer to those composite structures which are made up of different materials arranged in a certain sequence or according to some special replacement rules. Such layered periodic structures are often referred to as one-dimensional (1D) phononic crystals (PNCs). In analogy to the photonic crystals, the phononic crystals which were firstly introduced by Kushwaha et al. [1] represent new type of periodical functional structures, which exhibit elastic or acoustic band gaps. When the frequencies of elastic or acoustic waves are in the band gaps, the waves will be forbidden and cannot propagate through the structures. Due to this feature, the studies on PNCs are drawing more and more researchers' attentions. In particular, wave propagation in layered elastic structures or 1D PNCs has been investigated pretty comprehensively in the literature, because they are rather simpler than their two-dimensional (2D) and three-dimensional (3D) counterpart but still adequate to reveal the essential wave propagation phenomenon in PNCs. To cite an example, Golub et al. [2] investigated the anti-plane transverse wave (SH wave) propagation in periodically layered elastic composites with a damaged layer, and analyzed the influences of the damage types (periodic cracks and stochastic cracks approximated by distributed springs) on the wave field pattern and the band gaps.

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The periodic piezoelectric composite materials are of great practical importance in engineering applications. Baz [3] investigated the problems of active vibration control and wave localization in the periodic spring-mass systems controlled by the piezoelectric actuators, and Thorp et al. [4] studied the similar problem in the rods with the periodic shunted piezoelectric patches. Li and Wang et al. [5-7] presented the method for calculating the localization factor of the disordered periodic layered piezoelectric composite structures.

With the rapid development of the communication technology and biomedical engineering, the sizes of the devices are required to be smaller and smaller. For example, the communication tools operating at gigahertz usually need the nanoscale devices. The high frequency ultrasonic phononic band gaps are generally applied to design new thermo-electrical, acousto-optical, nanoscale electro-mechanical devices, etc. [8-10]. Thus, nanoscale structures have attracted a great deal of attentions in the scientific and engineering communities. Using the variational method with consideration of both surface elasticity and residual surface stress, Liu et al. [11] derived the critical detachment length from the transversality and discussed the influence of the surface parameters on the adhesion of a nano-beam. Alibeigloo [12] analyzed the vibration of a nano-plate based on three-dimensional theory of elasticity by using the non-local continuum mechanics. With the same method, Alibeigloo et al. [13] obtained the analytical solution for the bending of a simply supported rectangular graphene sheets. Ramprasad et al. [14] calculated the first two bands for the transverse wave propagating normally in a nanoscale $\text{HfO}_2\text{-ZrO}_2$ multilayer stack by using the first-principles methods at the atomistic level and by solving the acoustic wave equation at the continuum level, respectively. The result indicated the need for careful treatments when waves propagate through the nanoscale structures. Using a variety of atomic-level approaches rather than the traditional classical elastic continuum theory, Hepplestone [15] calculated the frequency gaps and negative group velocities of hypersonic phonon modes in periodically arranged composite semiconductors. Ke et al. [16] studied the nonlinear vibration of the piezoelectric nano-beams based on the nonlocal theory and Timoshenko beam theory. Chen and Wang et al. [17, 18] calculated the band structures for both anti-plane and in-plane elastic waves propagating normally or obliquely in nanoscale periodic layered structures by using the transfer matrix method based on the nonlocal elastic continuum theory [19, 20]. However, only few research works on the wave propagation in nanoscale periodic layered piezoelectric structures have been reported in literature due to the complexity of the problem. Therefore, it is needed to have a detailed study on this problem.

In this paper, the propagation and localization of the anti-plane transverse wave in the nanoscale periodic layered piezoelectric structure are studied. The transfer matrix method based on the nonlocal piezoelectricity (NLPE) continuum theory is used. Both the size effect and the electro-mechanical coupling effect are considered. The solutions of the equations of wave motion are derived. The dispersion curves and the localization factors are calculated to analyze the behaviors of the anti-plane transverse wave propagation in the nanoscale periodic layered piezoelectric structures. The

stiffness matrix method is also applied to compute the corresponding wave transmission spectra.

2. Nonlocal piezoelectricity theory and equations of wave motion

It is well known that in the classical piezoelectricity (CPE) theory, the stresses and the electric displacements at one point are only dependent on the local strains and electric fields at the same point. But when the macro size reaches a few nanometers, the CPE continuum theory fails and we have usually to utilize other methods. The nonlocal piezoelectricity (NLPE) continuum theory, as a commonly used method, supposes that the stresses and electric displacements at one point are affected by the strains and the electric fields at all points of the whole body, thus the constitutive relations can be written as [19, 20]

$$\tau_{mn}(\mathbf{x}) = \int_v \alpha(|\mathbf{x}' - \mathbf{x}|) T_{mn}(\mathbf{x}') dv(\mathbf{x}'), \quad (1a)$$

$$d_m(\mathbf{x}) = \int_v \alpha(|\mathbf{x}' - \mathbf{x}|) D_m(\mathbf{x}') dv(\mathbf{x}'), \quad (1b)$$

where $\mathbf{x}$ is the position vector; T_{mn} and D_m are the stress and electric displacement components calculated by the CPE theory, respectively; τ_{mn} and d_m are the nonlocal stress and electric displacement components, respectively. On the macroscopic scale, the constitutive equations are:

$$T_{mn} = c_{mnkl} S_{kl} - e_{kmn} E_k, \quad (2a)$$

$$D_m = e_{mkl} S_{kl} + v_{mk} E_k, \quad (2b)$$

where c_{mnkl} are the elastic constants; e_{mkl} are the piezoelectric constants and v_{mk} are the dielectric constants. The strain tensor $\mathbf{S}$ and the electric field vector $\mathbf{E}$ are related to the displacements u_m and the electric potential φ , by the following kinematic equations

$$S_{mn} = (u_{n,m} + u_{m,n}) / 2, \quad (3a)$$

$$E_m = -\varphi_{,m}. \quad (3b)$$

In Eq. (1) $\alpha(|\mathbf{x}' - \mathbf{x}|)$ is the influence function which can obtain the maximum at $\mathbf{x}' = \mathbf{x}$ and decrease with $|\mathbf{x}' - \mathbf{x}|$. It is closely related to the internal characteristic length ε (e.g. the atomic lattice constant). When $\varepsilon \rightarrow 0$, $\alpha(|\mathbf{x}' - \mathbf{x}|)$ reduces to the Dirac delta function $\delta(|\mathbf{x}' - \mathbf{x}|)$, and thus Eq. (1) reduces to the constitutive equations of CPE theory. More detailed information about the influence function α and its special forms can be found in Ref. [20].

As shown in Fig. 1, we consider a steady-state transverse wave polarized in the

z -direction propagating along the positive x -direction of a nanoscale periodic layered piezoelectric structure. The structure is composed of materials A and B with the thicknesses being a_1 and a_2 , respectively. Thus, $a=a_1+a_2$ is the thickness of the unit cell. It is noted that a_1 , a_2 and a are all on nanoscale. Since the structure is infinite along the y -direction, hence the influence function along the y -direction should be a Dirac delta function. Therefore the influence function can be written as

$$\alpha(|\mathbf{x}'-\mathbf{x}|)=\alpha(|x'-x|)\delta(|y'-y|), \quad (4)$$

with $\alpha(|x'-x|)$ being the influence function in the x -direction. In this analysis, we select the following explicit form of $\alpha(|x'-x|)$ [19, 20]:

$$\alpha(|x'-x|,\varepsilon)=\frac{1}{2\varepsilon}e^{-(|x'-x|/\varepsilon)}. \quad (5)$$

Then for the present 2D problem, the constitute relations, i.e. Eq. (1), can be rewritten as

$$\tau_{mn}(\mathbf{x})=\int_v \alpha(|\mathbf{x}'-\mathbf{x}|)T_{mn}(\mathbf{x}')dv(\mathbf{x}')=\int_{-\infty}^{+\infty}\int_0^a \alpha(|x'-x|)\delta(|y'-y|)T_{mn}(\mathbf{x}')dx'dy', \quad (6a)$$

$$d_m(\mathbf{x})=\int_v \alpha(|\mathbf{x}'-\mathbf{x}|)D_m(\mathbf{x}')dv(\mathbf{x}')=\int_{-\infty}^{+\infty}\int_0^a \alpha(|x'-x|)\delta(|y'-y|)D_m(\mathbf{x}')dx'dy', \quad (6b)$$

where a is the thickness of the unit cell.

The integral form of Eq. (6) can be approximated by the following differential ones [20]:

$$(1-\varepsilon^2\nabla^2)\tau_{mn}=T_{mn}, \quad (7a)$$

$$(1-\varepsilon^2\nabla^2)d_m=D_m, \quad (7b)$$

where $\nabla^2=\partial^2/\partial x^2+\partial^2/\partial y^2$ is the Laplace operator. The partial differential equations of motion without body forces are given as:

$$\tau_{mn,m}=\rho\ddot{u}_m, \quad (8a)$$

$$d_{m,m}=0, \quad (8b)$$

where ρ is the mass density, and the quasi-electrostatic assumption is made for the electric field.

In the case of anti-plane wave motion, the only non-zero mechanical displacement is u in the z -direction perpendicular to the xy -plane, and the remaining non-zero mechanical stress components are τ_{xz} and τ_{yz} . Substitution of Eqs. (2), (3) and (7) into Eq. (8), the anti-plane wave equations take the following forms:

$$c_{44}^{(j)}\nabla^2 u_j(x_j, y_j, t) + e_{15}^{(j)}\nabla^2 \varphi_j(x_j, y_j, t) = (1-\varepsilon_j^2\nabla^2)\rho_j\ddot{u}_j(x_j, y_j, t), \quad (9a)$$

$$e_{15}^{(j)}\nabla^2 u_j(x_j, y_j, t) - v_{11}^{(j)}\nabla^2 \varphi_j(x_j, y_j, t) = 0, \quad (9b)$$

where $j=1, 2$ stands for the j th sub-layer.

The time-harmonic solutions of the above equations are

$$u_j(x_j, y_j, t) = U_j(x_j) \exp[iky_j \sin \theta - i\omega t], \quad (10a)$$

$$\phi_j(x_j, y_j, t) = \Phi_j(x_j) \exp[iky_j \sin \theta - i\omega t], \quad (10b)$$

where $i^2=-1$; $k=\omega/c$ is the wavenumber of the incident wave; θ is the incidence angle; ω and c are the circular frequency and phase velocity, respectively; and U_j and Φ_j are the amplitudes of the displacements and the electric potentials, respectively.

Substituting Eq. (10) into Eq. (9) yields:

$$\frac{d^2 U_j}{dx_j^2} + k^2 \left(\frac{k_j^2}{k^2 - \varepsilon_j^2} - \sin^2 \theta \right) U_j = 0, \quad (11a)$$

$$\frac{d^2 \Phi_j}{dx_j^2} - k^2 \sin^2 \theta \Phi_j = p_j \left(\frac{d^2 U_j}{dx_j^2} - k^2 \sin^2 \theta U_j \right), \quad (11b)$$

where $p_j = e_{15}^{(j)} / v_{11}^{(j)}$ is the ratio of the piezoelectric constant to the dielectric constant of the piezoelectric materials; and $k_j=\omega/c_j$ are the wavenumbers with c_j being the phase velocities of the bulk shear waves of the piezoelectric materials determined by

$$c_j = \sqrt{\frac{[c_{44}^{(j)} v_{11}^{(j)} + (e_{15}^{(j)})^2]}{\rho_j v_{11}^{(j)}}}. \quad (12)$$

For convenience, we introduce the dimensionless local coordinates as:

$$\xi_j = \frac{x_j}{a}, \quad \eta_j = \frac{y_j}{a}, \quad (13)$$

where $\xi_j \in (0, \bar{a}_j)$, $\eta_j \in (0, +\infty)$, and $\bar{a}_j = a_j/a$ is the dimensionless thickness of the sub-layer. Then Eqs. (10) and (11) can be rewritten in dimensionless forms as:

$$u_j(\xi_j, \eta_j, t) = U_j(\xi_j) \exp[i\beta \eta_j \sin \theta - i\omega t], \quad (14a)$$

$$\phi_j(\xi_j, \eta_j, t) = \Phi_j(\xi_j) \exp[i\beta \eta_j \sin \theta - i\omega t], \quad (14b)$$

$$\frac{d^2 U_j}{d\xi_j^2} + \beta^2 \left(\frac{\beta_j^2}{\beta^2 - R_j^2} - \sin^2 \theta \right) U_j = 0, \quad (15a)$$

$$\frac{d^2 \Phi_j}{d\xi_j^2} - \beta^2 \sin^2 \theta \Phi_j = p_j \left(\frac{d^2 U_j}{d\xi_j^2} - \beta^2 \sin^2 \theta U_j \right), \quad (15b)$$

where $\beta=ka$ and $\beta_j=k_j a$ are the dimensionless wavenumbers; and $R_j=\varepsilon_j/a$ are the ratios of the internal to external characteristic lengths.

The general solutions of Eq. (15) can be obtained as:

$$U_j(\xi_j) = A_j \exp[-i q_j \xi_j] + B_j \exp[i q_j \xi_j], \quad (16a)$$

$$\Phi_j(\xi_j) = C_j \exp[-\beta \sin \theta \xi_j] + D_j \exp[\beta \sin \theta \xi_j] + p_j \{A_j \exp[-i q_j \xi_j] + B_j \exp[i q_j \xi_j]\}, \quad (16b)$$

where $q_j = \sqrt{\beta_j^2 / (1 - R_j^2 \beta_j^2) - \beta^2 \sin^2 \theta}$ are the dimensionless wavenumbers in the x -direction; and A_j, B_j, C_j and D_j are the unknown coefficients.

From Eqs.(2), (3), (5) and (16), we can obtain the stress and the electric displacement component as:

$$\begin{aligned} \tau_{xzj}(\xi_j) &= \int_0^{\bar{a}_j} \frac{1}{2R_j} e^{-\frac{|\xi_j - \xi'_j|}{R_j}} \left(c_{44}^{(j)} \frac{\partial u_j}{\partial \xi'_j} + e_{15}^{(j)} \frac{\partial \phi_j}{\partial \xi'_j} \right) d\xi'_j \\ &= -\frac{i q_j (c_{44}^{(j)} + e_{15}^{(j)} p_j)}{2} \left(\frac{e^{-i q_j \xi_j} - e^{-\xi_j/R_j}}{1 - i q_j R_j} - \frac{e^{-i q_j \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{-i q_j \xi_j}}{1 + i q_j R_j} \right) A_j \\ &\quad + \frac{i q_j (c_{44}^{(j)} + e_{15}^{(j)} p_j)}{2} \left(\frac{e^{i q_j \xi_j} - e^{-\xi_j/R_j}}{1 + i q_j R_j} - \frac{e^{i q_j \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{i q_j \xi_j}}{1 - i q_j R_j} \right) B_j \quad (17a) \end{aligned}$$

$$\begin{aligned} &- \frac{\beta \sin \theta e_{15}^{(j)}}{2} \left(\frac{e^{-\beta \sin \theta \xi_j} - e^{-\xi_j/R_j}}{1 - \beta \sin \theta R_j} - \frac{e^{-\beta \sin \theta \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{-\beta \sin \theta \xi_j}}{1 + \beta \sin \theta R_j} \right) C_j \\ &\quad + \frac{\beta \sin \theta e_{15}^{(j)}}{2} \left(\frac{e^{\beta \sin \theta \xi_j} - e^{-\xi_j/R_j}}{1 + \beta \sin \theta R_j} - \frac{e^{\beta \sin \theta \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{\beta \sin \theta \xi_j}}{1 - \beta \sin \theta R_j} \right) D_j, \\ d_{xj}(\xi_j) &= \int_0^{\bar{a}_j} \frac{1}{2R_j} e^{-\frac{|\xi_j - \xi'_j|}{R_j}} \left(e_{15}^{(j)} \frac{\partial u_j}{\partial \xi'_j} - \varepsilon_{11}^{(j)} \frac{\partial \phi_j}{\partial \xi'_j} \right) d\xi'_j \\ &= \frac{\beta \sin \theta \varepsilon_{11}^{(j)}}{2} \left(\frac{e^{-\beta \sin \theta \xi_j} - e^{-\xi_j/R_j}}{1 - \beta \sin \theta R_j} - \frac{e^{-\beta \sin \theta \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{-\beta \sin \theta \xi_j}}{1 + \beta \sin \theta R_j} \right) C_j \quad (17b) \\ &\quad - \frac{\beta \sin \theta \varepsilon_{11}^{(j)}}{2} \left(\frac{e^{\beta \sin \theta \xi_j} - e^{-\xi_j/R_j}}{1 + \beta \sin \theta R_j} - \frac{e^{\beta \sin \theta \bar{a}_j} e^{-(\bar{a}_j - \xi_j)/R_j} - e^{\beta \sin \theta \xi_j}}{1 - \beta \sin \theta R_j} \right) D_j. \end{aligned}$$

Form the above results, it can be seen that the parameter R_j and the ratio of the internal characteristic length ε_j to the unit cell length a , characterize the size effect at the nanoscale. When $R_j \rightarrow 0$ (i.e. $\varepsilon_j \rightarrow 0$), the solutions we have obtained from the NLPE theory are reduced to the results of the CPE theory.

3. Calculation of the transfer matrix and localization factor

We define $\mathbf{V} = \{\tau_{xz}, d_x, u, \phi\}^T$ as the state vector. Then the state vectors at the left and right sides of the j th sub-layer in the k th unit cell can be written as:

$$\mathbf{V}_{jL}^{(k)} = \{\tau_{xzj}, d_{xj}, u_j, \phi_j\}_{\xi_j=0}^T = \mathbf{M}_{jL} \{A_j, B_j, C_j, D_j\}^T, \quad (18a)$$

$$\mathbf{V}_{jR}^{(k)} = \{\tau_{xj}, d_{xj}, u_j, \phi_j\}_{\xi_j = \bar{a}_j}^T = \mathbf{M}_{jR} \{A_j, B_j, C_j, D_j\}^T, \quad (18b)$$

where $\mathbf{M}_{jL}$ and $\mathbf{M}_{jR}$ are 4×4 matrixes whose elements are given in Appendix A. According to Eq. (18), we have the following relationship:

$$\mathbf{V}_{jR}^{(k)} = \mathbf{M}_{jR} \mathbf{M}_{jL}^{-1} \mathbf{V}_{jL}^{(k)} \square \mathbf{N}_j \mathbf{V}_{jL}^{(k)}, \quad (19)$$

where $\mathbf{N}_j = \mathbf{M}_{jR} \mathbf{M}_{jL}^{-1}$ is the transfer matrix of the j th sub-layer.

The stresses, displacements, electric displacements and electric potentials are continuous at the interface between the k th and $(k-1)$ th unit cells and between the two sub-layers in a unit cell, i.e.,

$$\mathbf{V}_{1R}^{(k)} = \mathbf{V}_{2L}^{(k)}, \mathbf{V}_{1R}^{(k-1)} = \mathbf{V}_{2L}^{(k-1)}, \mathbf{V}_{2R}^{(k-1)} = \mathbf{V}_{1L}^{(k)}. \quad (20)$$

From Eqs. (18)- (20), the following relationships can be easily derived:

$$\mathbf{V}_{2R}^{(k)} = \mathbf{N}_2 \mathbf{V}_{2L}^{(k)} = \mathbf{N}_2 \mathbf{V}_{1R}^{(k)} = \mathbf{N}_2 \mathbf{N}_1 \mathbf{V}_{1L}^{(k)} = \mathbf{N}_2 \mathbf{N}_1 \mathbf{V}_{2R}^{(k-1)} \square \mathbf{T}_k \mathbf{V}_{2R}^{(k-1)}, \quad (21)$$

According to Eq. (21), the transfer relation between the two adjacent unit cells can be obtained as:

$$\mathbf{V}_{2R}^{(k)} = \mathbf{T}_k \mathbf{V}_{2R}^{(k-1)} \quad (k = 1, 2, \dots, n), \quad (22)$$

where $\mathbf{T}_k = \mathbf{N}_2 \mathbf{N}_1$ is the 4×4 transfer matrix between the two consecutive unit cells. Because of the periodicity, $\mathbf{T}_k$ for all $k=1, 2, \dots, n$ are the same and denoted as $\mathbf{T}$.

Considering the Bloch theorem [21], we have $\mathbf{V}_{2R}^{(k)} = e^{ik_x a} \mathbf{V}_{2R}^{(k-1)}$, and the following eigenvalue equation can be obtained from the transfer matrix $\mathbf{T}$ [22]

$$|\mathbf{T} - e^{ik_x a} \mathbf{I}| = 0, \quad (23)$$

where $\mathbf{I}$ is the unit matrix and k_x is the Bloch wave number in the x -direction. For a given ω , k_x can be found by solving the above eigenvalue equation. As long as k_x is real, the transverse wave at this frequency can propagate through the structure. On the contrary, if k_x is imaginary, this frequency is in the stop band or band gap where the wave is forbidden to propagate through the structure. Therefore, we can obtain the dispersion curves of the structure by solving Eq. (23).

The band structures of one-dimensional layered periodic structures can also be described by the localization factor [5-7], which is defined as the minimum positive Lyapunov exponent and describes the average exponential attenuation of the wave amplitudes when the acoustic or elastic waves propagate through the structure. The Lyapunov exponents can describe the dynamic behavior of a dynamical system quantitatively and qualitatively. Due to the symmetry of the periodic structure, Lyapunov exponents will always appear as pairs in the relationship of the mutual opportunity [23]. Assuming that the rank of the transfer matrix is $2m$, the Lyapunov exponents, i.e. the localization factors, γ_m , can be arranged as follows:

$$\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_m \geq 0 \geq \gamma_{m+1} (= -\gamma_m) \geq \gamma_{m+2} (= -\gamma_{m-1}) \geq \dots \geq \gamma_{2m} (= -\gamma_1). \quad (24)$$

In order to calculate the m th Lyapunov exponent, m orthogonal unit vectors of a dimension $2m$, $\mathbf{u}_1^{(0)}, \mathbf{u}_2^{(0)}, \dots, \mathbf{u}_m^{(0)}$, are chosen as the initial state vectors. Eq. (22) may be used to calculate the l th iteration

$$\mathbf{V}_{2R,j}^{(l)} = \mathbf{T}_{l+1} \mathbf{u}_j^{(l-1)} \quad (l = 1, 2, \dots, n; j = 1, 2, \dots, m), \quad (25)$$

where $\mathbf{u}_j^{(l-1)}$ are orthogonal unit vectors; while $\mathbf{V}_{2R,j}^{(l)}$ are usually not, and therefore they will be orthogonalized and normalized by following Gram-Schmidt orthonormalization procedure:

$$\begin{aligned} \hat{\mathbf{V}}_{2R,1}^{(l)} &= \mathbf{V}_{2R,1}^{(l)}, \mathbf{u}_1^{(l)} = \frac{\hat{\mathbf{V}}_{2R,1}^{(l)}}{\|\hat{\mathbf{V}}_{2R,1}^{(l)}\|}, \\ \hat{\mathbf{V}}_{2R,2}^{(l)} &= \mathbf{V}_{2R,2}^{(l)} - (\hat{\mathbf{V}}_{2R,2}^{(l)}, \mathbf{u}_1^{(l)}) \mathbf{u}_1^{(l)}, \mathbf{u}_2^{(l)} = \frac{\hat{\mathbf{V}}_{2R,2}^{(l)}}{\|\hat{\mathbf{V}}_{2R,2}^{(l)}\|}, \\ &\dots, \\ \hat{\mathbf{V}}_{2R,m}^{(l)} &= \mathbf{V}_{2R,m}^{(l)} - (\hat{\mathbf{V}}_{2R,m}^{(l)}, \mathbf{u}_{m-1}^{(l)}) \mathbf{u}_{m-1}^{(l)} - \dots - (\hat{\mathbf{V}}_{2R,m}^{(l)}, \mathbf{u}_1^{(l)}) \mathbf{u}_1^{(l)}, \mathbf{u}_m^{(l)} = \frac{\hat{\mathbf{V}}_{2R,m}^{(l)}}{\|\hat{\mathbf{V}}_{2R,m}^{(l)}\|}, \end{aligned} \quad (26)$$

where $(\bullet, \bullet)$ denotes the dot-product. Then based on Wolf's method [24], the localization factor γ_m may be obtained as:

$$\gamma_m = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{l=1}^n \|\hat{\mathbf{V}}_{2R,m}^{(l)}\|. \quad (27)$$

In this paper, the dimension of the transfer matrix is 4×4 . Therefore γ_2 is the corresponding localization factor, which is simply denoted by γ in the following discussion.

4. The stiffness matrix method

Usually, when the layer number is small or the frequency is relatively low, the transmission spectra calculated by the transfer matrix method are accurate and convergent. But if the structure involves many layers, especially when there is an evanescent wave in the periodic structure, the numerical results will be unstable and divergent. In order to eliminate this instability, the stiffness matrix method [25, 26] is introduced to calculate the transmission spectra.

Actually, the stiffness matrix method is a kind of conversion of the transfer matrix method. To derive the global stiffness matrix of the structure, we introduce the generalized stresses $\boldsymbol{\sigma} = \{\tau, d\}^T$ and the generalized displacements $\mathbf{u} = \{u, \varphi\}^T$. The stiffness matrices of the first and second layers in a unit cell are defined as $\mathbf{K}^A$ and $\mathbf{K}^B$. The generalized stresses and displacements at the left boundary of the first layer, at the interface between two sub-layers and at the right boundary of the second layer are denoted as $\{\boldsymbol{\sigma}_1, \mathbf{u}_1\}$, $\{\boldsymbol{\sigma}_2, \mathbf{u}_2\}$ and $\{\boldsymbol{\sigma}_3, \mathbf{u}_3\}$, respectively. Then we have the following expressions

$$\begin{bmatrix} \boldsymbol{\sigma}_1 \\ \boldsymbol{\sigma}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{11}^A & \mathbf{K}_{12}^A \\ \mathbf{K}_{21}^A & \mathbf{K}_{22}^A \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}, \quad (28)$$

$$\begin{bmatrix} \boldsymbol{\sigma}_2 \\ \boldsymbol{\sigma}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{11}^B & \mathbf{K}_{12}^B \\ \mathbf{K}_{21}^B & \mathbf{K}_{22}^B \end{bmatrix} \begin{bmatrix} \mathbf{u}_2 \\ \mathbf{u}_3 \end{bmatrix}. \quad (29)$$

Combining Eqs. (28) and (29), we can obtain the stiffness matrix of a unit cell as:

$$\begin{bmatrix} \boldsymbol{\sigma}_1 \\ \boldsymbol{\sigma}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{11}^A + \mathbf{K}_{12}^A (\mathbf{K}_{11}^B - \mathbf{K}_{22}^A)^{-1} \mathbf{K}_{21}^A & -\mathbf{K}_{12}^A (\mathbf{K}_{11}^B - \mathbf{K}_{22}^A)^{-1} \mathbf{K}_{12}^B \\ \mathbf{K}_{21}^B (\mathbf{K}_{11}^B - \mathbf{K}_{22}^A)^{-1} \mathbf{K}_{21}^A & \mathbf{K}_{22}^B - \mathbf{K}_{12}^B (\mathbf{K}_{11}^B - \mathbf{K}_{22}^A)^{-1} \mathbf{K}_{12}^B \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_3 \end{bmatrix} \quad (30)$$

Analogically, if we regard $\mathbf{K}^A$ as the global stiffness matrix $\mathbf{K}^{M-1}$ for the left $m-1$ unit cells, and $\mathbf{K}^B$ as the stiffness matrix $\mathbf{K}^m$ of the m th unit cell, then the global stiffness matrix $\mathbf{K}^M$ for a structure containing the left m unit cells can be defined as:

$$\mathbf{K}^M = \begin{bmatrix} \mathbf{K}_{11}^{M-1} + \mathbf{K}_{12}^{M-1} (\mathbf{K}_{11}^m - \mathbf{K}_{22}^{M-1})^{-1} \mathbf{K}_{21}^{M-1} & -\mathbf{K}_{12}^{M-1} (\mathbf{K}_{11}^m - \mathbf{K}_{22}^{M-1})^{-1} \mathbf{K}_{12}^m \\ \mathbf{K}_{21}^m (\mathbf{K}_{11}^m - \mathbf{K}_{22}^{M-1})^{-1} \mathbf{K}_{21}^{M-1} & \mathbf{K}_{22}^m - \mathbf{K}_{12}^m (\mathbf{K}_{11}^m - \mathbf{K}_{22}^{M-1})^{-1} \mathbf{K}_{12}^m \end{bmatrix} \quad (31)$$

Assume that both sides of the structure as shown in Fig. 1 are half-planes. For the anti-plane transverse wave propagating with arbitrary degree θ , the wave fields in the incident half-plane can be described by:

$$u_0 = U_0 \exp[i q_0 \xi_0] + U_1 \exp[-i q_0 \xi_0], \quad (32a)$$

$$\phi_0 = \Phi_1 \exp[\beta \sin \theta \xi_0], \quad (32b)$$

where U_0 , U_1 and Φ_1 are the amplitudes of the incident displacement, the reflected displacement and the reflected electric potential, respectively. Similarly, the wave field in the transmission half-plane can be described by:

$$u_m = U_m \exp[i q_m \xi_m], \quad (33a)$$

$$\phi_m = \Phi_m \exp[\beta \sin \theta \xi_m], \quad (33b)$$

where U_m and Φ_m are the amplitudes of the transmitted displacement and electric potential, respectively, and the incident and transmitted dimensionless wavenumbers are given by

$$q_0 = \sqrt{\beta_0^2 / (1 - R^2 \beta_0^2) - \beta^2 \sin^2 \theta}, \quad q_m = \sqrt{\beta_m^2 / (1 - R^2 \beta_m^2) - \beta^2 \sin^2 \theta},$$

with 0 and m representing the left and right half-plane of the structure, respectively. The incident and transmission state vectors are $\boldsymbol{\sigma}_0 = \{ \tau_{xz0}, d_{x0} \}^T$, $\mathbf{u}_0 = \{ u_0, \phi_0 \}^T$, and $\boldsymbol{\sigma}_m = \{ \tau_{xzm}, d_{xm} \}^T$, $\mathbf{u}_m = \{ u_m, \phi_m \}^T$, respectively. And they have the following relationship:

$$\begin{bmatrix} \boldsymbol{\sigma}_0 \\ \boldsymbol{\sigma}_m \end{bmatrix} = \mathbf{K}^M \begin{bmatrix} \mathbf{u}_0 \\ \mathbf{u}_m \end{bmatrix}. \quad (34)$$

Substituting Eqs. (32) and (33) into Eq. (34), we can obtain the transmission and reflection coefficients as:

$$\begin{bmatrix} \frac{U_m}{U_0}, \frac{\Phi_m}{U_0}, \frac{U_1}{U_0}, \frac{\Phi_1}{U_0} \end{bmatrix} = \mathbf{M}^{-1} \mathbf{b}, \quad (35)$$

where U_m/U_0 , Φ_m/U_0 are the transmission coefficients, and U_1/U_0 , Φ_1/U_0 are the reflection coefficients. The elements of the matrix $\mathbf{M}$ and the vector $\mathbf{b}$ are given in Appendix B.

5. Numerical results and discussions

In this section, numerical results are presented and discussed. The materials of layers A and B are polymer and piezoelectric ceramic, respectively. The material constants used in this paper are listed in Table 1. Unless otherwise stated, the materials are Polythene and PZT-5H during calculations. The thickness of each layer is assumed to be the same, i.e. $a_1 = a_2$. The internal characteristic lengths ε_1 and ε_2 of the two materials are assumed to have the same value $\varepsilon_1 = \varepsilon_2 = \varepsilon$. Then we have $R_1 = R_2 = R$.

For convenience, the frequency is normalized as $\Omega_{T1} = \omega a / c_{T1}$ with $c_{T1} = \sqrt{c_{44}^{(1)} / \rho_1}$.

5.1 Normal incidence

First, the propagation behaviors of the anti-plane transverse wave incident normally in the nanoscale periodic layered piezoelectric structure are studied. The localization factors varying with the normalized frequency Ω_{T1} for $R=0$ and $R=0.09$ are shown in Fig. 2. It should be noticed that the nanoscale size effect is considered for $R \neq 0$. The frequency ranges are pass bands in which the localization factors are zero, and the frequency ranges are band gaps in which the localization factors are positive. From Fig. 2, we can easily find that the band structures for $R=0$ and $R=0.09$ have a great difference. For $R=0.09$, the first band gap becomes a little lower and narrower, followed by many narrow band gaps. In this case, the localization factors are very big, which means a very strong wave localization phenomenon. At $\Omega_{T1}=5.556$, the localization factor reaches the first peak value, and then two wider band gaps appear, followed again by multiple narrow band gaps with very large localization factors. The second peak of the localization factors appears at $\Omega_{T1}=11.263$ beyond which the localization factors are not oscillating with a large value, meaning that the transverse wave over this frequency cannot propagate through the structure. This frequency is indeed a cut-off frequency. It is noted that no cut-off frequency exists for $R=0$.

To verify the accuracy of the band structures described by the localization factors, we calculate the displacement transmission coefficients for a finite structure with 40 layers as shown by the gray solid lines in Fig. 3. The red dashed lines in Fig. 3 are the displacement transmission coefficients estimated by the localization factors. It can be seen that the displacement transmission coefficients for a finite structure with 40 layers oscillate near the values estimated by the localization factors. The results estimated by the localization factors are a little bigger than those calculated by the stiffness method except at some peaks. This is due to the fact that the localization

factors describe the propagating wave with the weakest attenuation. Generally, the localization factor can give a satisfying evaluation of the displacement transmission. Furthermore, the band gaps and pass bands described by the two methods are in a good agreement for both cases of $R=0$ and $R=0.09$.

The dispersion curves calculated by Eq. (23) are given in Fig. 4. The black solid dots and red hollow dots stand for $R=0$ and $R=0.09$, respectively. Compared with Fig. 2, it is not difficult to see that the band structures described by the localization factors are consistent with the dispersion curves. For instance, the dispersion curves for $R=0.09$ shown in Fig. 4 disappear when the normalized frequency $\Omega_{T1} \geq 11.263$. And $\Omega_{T1}=11.263$ is just the cut-off frequency shown in Fig. 2. Additionally, near $\Omega_{T1}=5.556$ the bands are very dense and almost flat, which means a strong wave localization phenomenon in this frequency range. This is in a good agreement with that described by the localization factors in Fig. 2.

Then, we discuss the piezoelectric effect and the nanoscale size effect. The influence of the piezoelectricity on the band structures for $R=0$ is presented firstly in the Fig. 5(a), which shows an extremely complex feature, especially in the high frequency ranges. Generally, the first two band gaps are of special importance for applications, to which more attention should be paid. By combining Fig. 5(a) and Fig. 5(b), which is more evident, we can easily see that the band gap widths increase with the increase of the piezoelectric constant. The lower edges of the band gaps remain almost unchanged, and the upper edge of the second band gap is shifted much more to high frequencies than the first one. The bigger the piezoelectric constant is, the stronger the wave localization phenomenon is. For a further view, we discuss the effect of the piezoelectric constant and take the nanoscale size effect into account for $R=0.09$ in Fig. 6. It can be seen that the piezoelectricity has a similar effect as for $R=0$ in the low frequency ranges, and more importantly, the cut-off frequencies increase with the increase of the piezoelectric constant.

Fig. 7 shows the influence of the nanoscale size effect on the localization factors. The ratios of the internal and external characteristic lengths are taken as $R=0, 0.0225, 0.045, 0.09$ and 0.18 , respectively. It can be seen that the tendency of all curves is similar for all cases of $R \neq 0$: a cut-off frequency appears, beyond which the localization factors become free of oscillation with a large value. Near the cut-off frequency there is a range where the values of the localization factors oscillate quickly. Moreover, the cut-off frequencies decrease with the increase of R . Fig. 8 illustrates the variation of the normalized cut-off frequency with the values of R in details. The decrease of the cut-off frequency follows closely the increase of R . This implies that we can adjust the cut-off frequency by changing the thickness of the layers or the internal characteristic length ε .

Next, the influence of the impedance ratio on the band structure of the system is discussed. Here, we select four material combinations: $\text{CoFe}_2\text{O}_4/\text{PZT-4}$, $\text{PVDF}/\text{BaTiO}_3$, $\text{Graphite-epoxy}/\text{PZT-5A}$ and $\text{Polythene}/\text{PZT-5H}$. The corresponding material parameters are given in Table 1. The impedance ratios are chosen as $Z=\rho_2 c_{T2}/\rho_1 c_{T1}=1.097, 5.060, 7.295$ and 12.885 , respectively. The variation of the localization factors with the normalized frequency is shown in Fig. 9 for $R=0.09$. As

the impedance ratio increases, the main band gaps in the low frequency ranges (generally, $\Omega_{T1} \leq 5.556$) become wider and shifted to the low frequencies. For instance, with the increase of the impedance ratio, the first band gap (2.399, 2.867) in Fig. 9(a), moves to (1.283, 2.538), (1.070, 2.586) and (0.959, 2.673). It can be also seen that with the increase of the impedance ratio, the frequencies of the first peak remain almost unchanged and the corresponding values of the localization factors rise slightly. While at the second peak points, i.e. the cut-off frequency points, the values of the non-oscillating localization factor go up and the cut-off frequencies increase. Either near the first peak points or the second ones, there always exists a very strong wave localization phenomenon.

5.2 Oblique incidence

The localization factors for the transverse wave incident at an angle of 25° for $R=0$ and $R=0.09$ are calculated and the results are shown in Fig. 10. The corresponding displacement transmission coefficients of a finite structure with 40 layers are also computed. The results from the stiffness matrix method (the gray solid lines) and the localization factors (the red dash lines) are illustrated in Fig. 11. Similar to the normal incidence, we can easily see that the band structures described by the two methods have a good agreement as for the oblique incidence. So it validates again the accuracy and the feasibility of both methods to study the band structures for the oblique wave incidence.

The gray scale maps in Fig. 12 describe the localization factors varying with $k_y = \beta \sin \theta$ and the normalized frequency under the cut-off frequency for the transverse waves propagating with an arbitrary incidence angle. The white areas are pass bands and the gray areas are band gaps. It can be seen that all bands are compressed under the cut-off frequency with the increase of R . The band gaps become wider with pass bands becoming narrower. But R has only a little influence on the low frequency band structure. The pass bands will intersect with the increase of k_y which is marked by the three dashed circles in Fig. 12(b). Near the cut-off frequency, the pass bands become extremely narrow. That is to say, the localization phenomenon is rather strong in these ranges. Additionally, the values of the cut-off frequency are almost equal to those in the case of normal incidence.

6. Conclusions

In the present work, the propagation and localization of both normally and obliquely incident transverse waves in nanoscale periodic layered piezoelectric structures are studied. The NLPE continuum theory is utilized to take the size effect into account. The localization factor is introduced to describe the band structures. The dispersion curves and the corresponding transmission spectra are computed as well. The influences of the size effect, the piezoelectric constant and the impedance ratio on the cut-off frequency and the wave propagation behavior are analyzed and discussed. The essential conclusions from the present numerical results are drawn as follows:

- 1) When taking the nanoscale size effect into consideration, a cut-off frequency will appear beyond which elastic waves cannot propagate through the structure. With the increase of R as the ratio of the internal to external characteristic lengths, the

cut-off frequency decreases and the non-oscillating value of the localization factors goes down. On the other hand, the nonlocal effect has only a little influence in the low frequency ranges.

- 2) With the increase of the piezoelectric constant e_{15} , the first two band gaps become wider and wider. And the cut-off frequency increases with the increase of the piezoelectric constant.
- 3) The frequencies at the first peak point do not change with the impedance ratio. The values of the cut-off frequency and the non-oscillating localization factors increase as the impedance ratio increases.
- 4) For oblique wave incidence all bands are compressed under the cut-off frequency. Near the cut-off frequency, the bands are very dense and flat, which indicates a strong wave localization phenomenon.

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Appendix A

For transverse waves propagating in nanoscale periodic layered piezoelectric structures, the matrices $\mathbf{M}_{jL}$ and $\mathbf{M}_{jR}$ in Eq. (18) can be written as:

$$\mathbf{M}_{jL} = \begin{bmatrix} \frac{-iq_j(c_{44}^{(j)} + e_{15}^{(j)}p_j)(1 - e^{-iq_j\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 + iq_jR_j)} & \frac{iq_j(c_{44}^{(j)} + e_{15}^{(j)}p_j)(1 - e^{iq_j\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 - iq_jR_j)} & \frac{-e_{15}^{(j)}k_y(1 - e^{-k_y\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 + k_yR_j)} & \frac{e_{15}^{(j)}k_y(1 - e^{k_y\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 - k_yR_j)} \\ 0 & 0 & \frac{v_{11}^{(j)}k_y(1 - e^{-k_y\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 + k_yR_j)} & \frac{-v_{11}^{(j)}k_y(1 - e^{k_y\bar{a}_j}e^{-\bar{a}_j/R_j})}{2(1 - k_yR_j)} \\ 1 & 1 & 0 & 0 \\ p_j & p_j & 1 & 1 \end{bmatrix},$$

$$\mathbf{M}_{jR} = \begin{bmatrix} \frac{-iq_j(c_{44}^{(j)} + e_{15}^{(j)}p_j)(e^{-iq_j\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 - iq_jR_j)} & \frac{iq_j(c_{44}^{(j)} + e_{15}^{(j)}p_j)(e^{iq_j\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 + iq_jR_j)} & \frac{-e_{15}^{(j)}k_y(e^{-k_y\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 - k_yR_j)} & \frac{e_{15}^{(j)}k_y(e^{k_y\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 + k_yR_j)} \\ 0 & 0 & \frac{v_{11}^{(j)}k_y(e^{-k_y\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 - k_yR_j)} & \frac{-v_{11}^{(j)}k_y(e^{k_y\bar{a}_j} - e^{-\bar{a}_j/R_j})}{2(1 + k_yR_j)} \\ e^{-iq_j\bar{a}_j} & e^{iq_j\bar{a}_j} & 0 & 0 \\ p_j e^{-iq_j\bar{a}_j} & p_j e^{iq_j\bar{a}_j} & e^{-k_y\bar{a}_j} & e^{k_y\bar{a}_j} \end{bmatrix}.$$

Appendix B

For calculating the wave transmission spectra by the stiffness matrix method, the matrix $\mathbf{M}$ and the vector $\mathbf{b}$ in Eq. (35) can be written as:

$$\mathbf{M} = \begin{bmatrix} K^M(1,3) + p_m K^M(1,4) & K^M(1,4) & K^M(1,1) + p_0 K^M(1,2) + i q_0 (c_{44}^{(0)} + e_{15}^{(0)} p_0) & K^M(1,2) + e_{15}^{(0)} k_y \\ K^M(2,3) + p_m K^M(2,4) & K^M(2,4) & K^M(2,1) + p_0 K^M(2,2) & K^M(2,2) - v_{15}^{(0)} k_y \\ K^M(3,3) + p_m K^M(3,4) - i q_m (c_{44}^{(m)} + e_{15}^{(m)} p_m) & K^M(3,4) - e_{15}^{(m)} k_y & K^M(3,1) + p_0 K^M(3,2) & K^M(3,2) \\ K^M(4,3) + p_m K^M(4,4) & K^M(4,4) + v_{15}^{(m)} k_y & K^M(4,1) + p_0 K^M(4,2) & K^M(4,2) \end{bmatrix},$$

$$\mathbf{b} = [i q_0 (c_{44}^{(0)} + e_{15}^{(0)} p_0) - K^M(1,1) - p_0 K^M(1,2), -K^M(2,1) - p_0 K^M(2,2), -K^M(3,1) - p_0 K^M(3,2), -K^M(4,1) - p_0 K^M(4,2)]^T.$$

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Table captions

Table 1. Material constants of the polymers and piezoelectric ceramics

Figure captions

Figure 1. Schematic diagram of a nanoscale periodic layered piezoelectric structure

Figure 2. Localization factors varying with the normalized frequency. The black and red solid lines represent the results for $R=0$ and $R=0.09$, respectively.

Figure 3. The displacement transmission coefficients for a structures with 40 layers calculated by the stiffness method (the gray solid lines) and estimated by the localization factors (the red dash lines) for (a) $R=0$ and (b) $R=0.09$, respectively.

Figure 4. Dispersion curves for the transverse wave propagating normally in the nanoscale periodic layered structures. Black solid and red hollow dots stand for $R=0$ and $R=0.09$, respectively.

Figure 5. (a) Influences of the piezoelectric constant $e_{15}^{(2)}$ on the localization factors for $R=0$; and (b) the lower (the black solid lines) and upper (the red solid lines) edges of the first two band gaps varying with $e_{15}^{(2)}$.

Figure 6. Influences of the piezoelectric constant $e_{15}^{(2)}$ on the localization factors for $R=0.09$.

Figure 7. Influences of R on the localization factors with the black dotted line and colored solid lines for $R=0$ and $R \neq 0$, respectively.

Figure 8. Influences of R on the cut-off frequency for the normal incidence.

Figure 9. Influences of the impedance ratio on the localization factors for $R=0.09$ in the case of normal incidence.

Figure 10. Localization factors varying with the normalized frequency for the transverse wave incident at an angle of 25° for $R=0$ (the black lines) and $R=0.09$ (the red lines), respectively.

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Table 1. Material constants of the polymers and piezoelectric ceramics

Materials	Elastic constant c_{44} [10^9 N/m ²]	Mass density ρ [10^3 Kg/m ³]	Piezoelectric constant e_{15} [C/m ²]	Dielectric constant ϵ_{11} [10^{-9} N/m]
Polythene ^[5]	1.28	1.18	0.0	0.02036
PZT-5H ^[5]	23.0	7.50	17.0	27.7
PVDF ^[6]	7.0	1.78	0.0	0.06726
PZT-4 ^[27]	25.6	7.60	12.72	13.06
CoFe ₂ O ₄ ^[27]	45.3	5.30	0.0	0.08
BaTiO ₃ ^[27]	43.0	5.8	11.6	11.2
Graphite-epoxy ^[27]	2.87	1.59	0.0	15.3
PZT-5A ^[27]	21.1	7.75	12.322	15.3