

A continuum model with microstructures for wave propagation in ultra-thin films

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Abstract

Ultrasonic waves are powerful and popular methods for measuring mechanical properties of solids even at nanoscales. The extraction of material constants from the measured wave data requires the use of a model that can accurately describe the wave motion in the solid. The objective of this paper is to develop a continuum theory with microstructures that can capture the effect of the microstructure or nanostructure in ultra-thin films when waves of short wavelengths are used. This continuum theory is developed from assumed displacement fields for microstructures. Local kinematic variables are introduced to express these local displacements and are subjected to internal continuity conditions. The accuracy of the present theory is verified by comparing the results with those of the lattice model for the thin film. Specifically, dispersion curves for surface wave propagation and wave propagation in a thin film supported by an elastic homogeneous substrate are studied. The inadequacy of the conventional continuum theory is discussed.

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1. Introduction

Thin films used in microelectronic and microelectromechanical systems (MEMS) are getting thinner and their thickness is now reaching nanoscale. The mechanical and physical properties of these ultra-thin films may be quite different from those of their bulk counterparts. Testing the mechanical properties of ultra-thin films has gained much attention recently (Freund and Suresh, 2003; Schneider et al., 2000; Zhao et al., 2005). A number of methods for testing properties of thin film materials have been proposed including nanoindentation (Lee et al., 2004) and bulge testing (Li and Cima, 2004). Among the methods that have been used the acoustic wave technique has proved to be an efficient nondestructive method for testing material properties of thin films, especially for ultra-thin films. Hernaandez et al. (2002) used narrow band guided acoustic high-frequency waves excited by a two crossed laser beam to estimate the in-plane mechanical properties of

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silicon nitride membranes. The mechanical properties and residual stresses in the membranes were evaluated from the measured acoustic dispersion curves. The mean values of the Young's modulus and density of three nanocrystalline diamond films and a free standing diamond plate were determined by analyzing the dispersion of laser-generated surface waves (Philip et al., 2003). Ultra-thin films of 5–30 nm were investigated by Schneider et al. (2000) who used the laser-acoustic technique to measure the dispersion of surface acoustic waves. According to this study, higher frequency waves were needed for thinner films. Recently, high-frequency (THz) mechanical bulk waves were employed to determine material properties or thicknesses of thin membranes in nanometer scale (Vollmann et al., 2004; Profunser et al., 2004). In the studies above, the material properties were derived from the measured phase velocity using the conventional continuum model. The effect of nanostructures on high-frequency wave propagation has not been taken into consideration.

It has been recognized that classical continuum models could become inadequate in describing the response of solids when the characteristic length (or wave length) of deformation becomes comparable to or smaller than the characteristic length of microstructures in the solid. Since the Cosserat's model (1909) was introduced, there have been different versions of continuum theories with microstructures proposed by different authors (Toupin, 1962; Mindlin, 1964; Eringen and Suhubi, 1964). In these theories, special kinematic variables were introduced to describe the local motion of microstructures. However, the large number of material constants were left undetermined, which would require rather prohibitive experiments. Recently, Chen et al. (2003) and Chen and Lee (2003a,b) have attempted to determine the material constants in the micromorphic theory (Eringen, 1999) by relating the micromorphic theory to atomistic models.

Another approach toward developing a continuum theory was taken by a number of authors who considered the exact configuration of the local structure in the system. By employing several kinematic variables to describe the local motion in addition to the macro-kinematic variables, continuum models with microstructures were derived (Sun et al., 1968; Achenbach et al., 1968) for periodically layered systems. The main advantage of this approach is that the material constants in the resulting continuum model are obtained directly from the original material system without ambiguity. Muhlhaus and Oka (1996) developed a continuum theory by a direct homogenization of the discrete equations of motion for granular materials. Frieseche and James (2000) proposed a scheme based on the affine deformation of atoms to build a passage from atomic level to continuum level. This model is suitable only for static cases. Wang and Sun (2002) introduced a continuum model with micro inertia that retains the simplicity of the classical continuum mechanics while capturing the characteristics of the microstructure.

In the present paper, we employ a procedure similar to that of Sun et al. (1968) to develop a continuum model with microstructures based on the atomic structure of ultra-thin films. The atomistic crystal structure of the thin film, for the sake of simplicity, is represented by a lattice model. The dimensions of the crystal structure naturally appear in the constitutive equations and the equations of motion of the representative continuum. The accuracy of the present model is evaluated by comparing dispersions of free harmonic waves predicted by the continuum model and exact analysis based on the lattice model.

2. Continuum model for ultra-thin films

A thin film of cubic structure as shown in Fig. 1 is considered. The thin film has a uniform thickness h and is assumed to be in a state of plane strain parallel to the X_1 – X_3 plane. The discrete solid dots denote atoms m_1

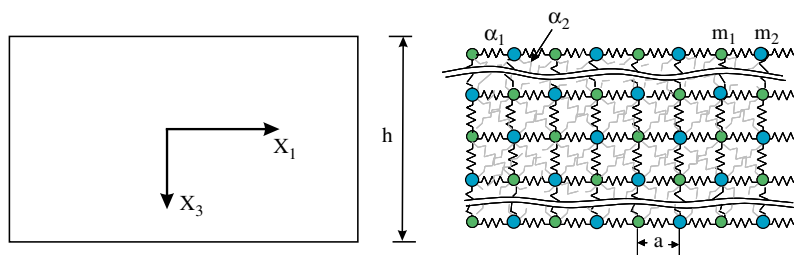


Fig. 1. Thin film structure and its lattice system.

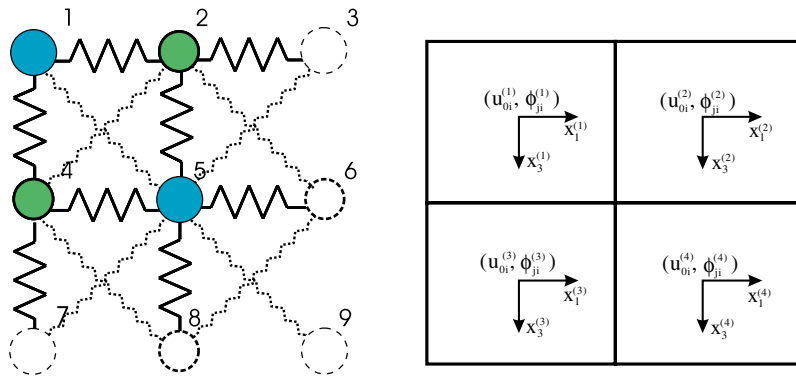


Fig. 2. Representative unit cell and the equivalent continuum.

and m_2 . The spacing between two adjacent atoms is a . Only the interactions between the nearest and next-nearest neighbors are considered. By assuming infinitesimal deformations, the interactions are represented by linearly elastic springs with spring constants α_1 and α_2 , respectively (Ghatak and Kothari, 1972). Although the cubic structure is chosen for the sake of mathematical simplicity, the proposed approach can be readily applied for thin films with other crystal structures.

A representative unit cell (see Fig. 2) of the cubic lattice model is considered in this study. The representative cell is composed of four sub-cells. In each sub-cell, a local coordinate system is set up as shown in Fig. 2. Note that in this representative element, atoms 3, 6, 7, 8, and 9 are not included in the representative cell because they are included in the adjacent cells. The four local coordinate systems $(x_1^{(k)}, x_3^{(k)})$ with origins located at the geometrical centers of the four sub-cells ($k = 1-4$), respectively, are set up so that x_1 and x_3 are parallel to the global (macro) coordinates X_1 and X_3 , respectively.

The local displacements $u_i^{(k)}$ in each sub-element are expanded in power series with respect to the respective local coordinates as

$$u_i^{(k)} = u_{0i}^{(k)} + \phi_{1i}^{(k)} x_1^{(k)} + \phi_{3i}^{(k)} x_3^{(k)}, \quad k = 1, 2, 3, 4, \quad (1)$$

where the expansion is truncated at the linear terms. Greater accuracy may be achieved by adding higher order terms in Eq. (1). We assume that local translational displacements $u_{0i}^{(k)}$ of the four sub-cells are values of macrodisplacement U_i at the four sub-cells, respectively, i.e.,

$$\begin{aligned} u_{0i}^{(1)}(X_1, X_3) &= U_i(X_1, X_3), \\ u_{0i}^{(2)} &= U_i(X_1 + a, X_3) \approx U_i(X_1, X_3) + a \frac{\partial U_i}{\partial X_1}, \\ u_{0i}^{(3)} &= U_i(X_1, X_3 + a) \approx U_i(X_1, X_3) + a \frac{\partial U_i}{\partial X_3}, \\ u_{0i}^{(4)} &= U_i(X_1 + a, X_3 + a) \approx U_i(X_1, X_3) + a \frac{\partial U_i}{\partial X_1} + a \frac{\partial U_i}{\partial X_3}. \end{aligned} \quad (2)$$

The kinematic variables $u_{0i}^{(k)}$, $\phi_{1i}^{(k)}$, and $\phi_{3i}^{(k)}$ are required to satisfy the displacement continuity conditions along the boundaries shared by the adjacent pairs of the sub-cells. These boundary conditions lead to the following relations:

$$[\phi_{ji}^{(2)}] = \begin{bmatrix} 2 \frac{\partial U_1}{\partial X_1} - \Phi_{11} & 2 \frac{\partial U_3}{\partial X_1} - \Phi_{13} \\ \Phi_{31} & \Phi_{33} \end{bmatrix}, \quad (3)$$

$$[\phi_{ji}^{(3)}] = \begin{bmatrix} \Phi_{11} & \Phi_{13} \\ 2 \frac{\partial U_1}{\partial X_3} - \Phi_{31} & 2 \frac{\partial U_3}{\partial X_3} - \Phi_{33} \end{bmatrix}, \quad (4)$$

$$[\phi_{ji}^{(4)}] = \begin{bmatrix} 2 \frac{\partial U_1}{\partial X_1} - \Phi_{11} & 2 \frac{\partial U_3}{\partial X_1} - \Phi_{13} \\ 2 \frac{\partial U_1}{\partial X_3} - \Phi_{31} & 2 \frac{\partial U_3}{\partial X_3} - \Phi_{33} \end{bmatrix} \quad (5)$$

in which

$$\Phi_{ji}(X_1, X_3) \equiv \phi_{ji}^{(1)}(X_1, X_3). \quad (6)$$

The deformation energy in each sub-cell can be written as

$$W^{(1)} = W_{1-2} + W_{1-4} + W_{1-5} + W_{2-4}, \quad (7)$$

$$W^{(2)} = W_{2-3} + W_{2-5} + W_{2-6} + W_{3-5}, \quad (8)$$

$$W^{(3)} = W_{4-5} + W_{4-7} + W_{4-8} + W_{5-7}, \quad (9)$$

$$W^{(4)} = W_{5-6} + W_{5-8} + W_{5-9} + W_{6-8}, \quad (10)$$

where superscripts 1, 2, 3, and 4 represent the sub-cells, and W_{1-2} , $W_{1-5} \dots$ denote the total deformation energies due to stretching of the springs between atoms 1 and 2 and 1 and 5 ..., respectively. Detailed derivations for W_{1-2} and W_{1-5} are presented in the following to illustrate the procedure. Other terms can be obtained in a similar manner.

Consider the deformation energy W_{1-2} between atoms 1 and 2. The displacements of atom 2 may be taken from sub-cell 1 or sub-cell 2. For simplicity, we take the displacements for both atoms 1 and 2 from sub-cell 1. We have

$$W_{1-2} = \frac{1}{2} \alpha_1 \left[\sqrt{(a + {}_2u_1^{(1)} - {}_1u_1^{(1)})^2 + ({}_2u_3^{(1)} - {}_1u_3^{(1)})^2} - a \right]^2 = \frac{1}{2} \alpha_1 \left[\sqrt{(a + \phi_{11}^{(1)})^2 + (\phi_{31}^{(1)})^2} - a \right]^2, \quad (11)$$

where ${}_p u_i^{(k)}$ represents displacement component u_i in sub-cell k at atom p . Using the binomial expansion and taking the first two terms we have

$$W_{1-2} = \frac{1}{2} \alpha_1 (a \phi_{11}^{(1)})^2. \quad (12)$$

In a similar manner, we can express the deformation energy between atoms 1 and 5 as

$$W_{1-5} = \frac{1}{2} \alpha_2 \left[\sqrt{(a + {}_5u_1^{(1)} - {}_1u_1^{(1)})^2 + (a + {}_5u_3^{(1)} - {}_1u_3^{(1)})^2} - \sqrt{2}a \right] = \frac{1}{4} \alpha_2 (\phi_{11}^{(1)} + \phi_{31}^{(1)} + \phi_{13}^{(1)} + \phi_{33}^{(1)})^2. \quad (13)$$

The total deformation energy in sub-cell 1 is

$$W^{(1)} = \frac{1}{2} \alpha_1 a^2 [(\phi_{11}^{(1)})^2 + (\phi_{33}^{(1)})^2] + \frac{1}{4} \alpha_2 (\phi_{11}^{(1)} + \phi_{31}^{(1)} + \phi_{13}^{(1)} + \phi_{33}^{(1)})^2 + \frac{1}{4} \alpha_2 (\phi_{11}^{(1)} - \phi_{31}^{(1)} - \phi_{13}^{(1)} + \phi_{33}^{(1)})^2. \quad (14)$$

The deformation energies for other sub-cells have a similar expression as Eq. (14).

Based on the continuity conditions of displacements, Eqs. (3)–(5) the kinematic variables $\phi_{ji}^{(k)}$ ($j, i = 2, 3, 4$) in sub-cells 2, 3, and 4 can be eliminated and expressed in terms of the kinematic variables of sub-cell 1. Thus, the total deformation energy stored in the representative unit cell (that consists of four sub-cells) can be expressed in terms of U_i and Φ_{ji} and their derivatives. By dividing this total energy with the planar area $4a^2$ we obtain the strain energy density W of the representative cell after some manipulations. We have

$$\begin{aligned} W &= \frac{1}{4a^2} (W^{(1)} + W^{(2)} + W^{(3)} + W^{(4)}) \\ &= \frac{1}{2} \alpha_1 (E_{11}^2 + E_{33}^2 + \gamma_{11}^2 + \gamma_{33}^2) + \frac{1}{2} \alpha_2 [(E_{11} + E_{33})^2 + \gamma_{11}^2 + \gamma_{33}^2 + \gamma_{13}^2 + \gamma_{31}^2 + 4E_{13}^2], \end{aligned} \quad (15)$$

where

$$E_{ij} = \frac{1}{2} (U_{i,j} + U_{j,i}), \quad i, j = 1, 3 \quad (16)$$

is the macrostrain and

$$\gamma_{ji} = U_{j,i} - \Phi_{ji}, \quad i, j = 1, 3 \quad (17)$$

is the relative strain. These two deformation variables resemble those in Mindlin's microstructure theory (Mindlin, 1964). This strain energy density function forms the base of the continuum model that represents the discrete lattice system.

To establish the constitutive relations we define Cauchy stress

$$\Sigma_{ij} = \frac{\partial W}{\partial E_{ij}} \quad (18)$$

and relative stress

$$\sigma_{ij}^R = \frac{\partial W}{\partial \gamma_{ij}}. \quad (19)$$

It is noted that if γ_{ij} is absent, then the relative stress σ_{ij}^R vanishes, and the strain energy density function reduces to that of the classical continuum. This reduced model will be referred to as the “effective modulus” theory.

The kinetic energy density function for the representative cell of the thin film can be derived from the discrete system based on the local displacements given by Eq. (1). We obtain

$$\begin{aligned} T = & \frac{m_1}{4a^2} \left[\dot{U}_1^2 + \dot{U}_3^2 + \frac{a^2}{4} (\dot{\Phi}_{11} + \dot{\Phi}_{31})^2 + \frac{a^2}{4} (\dot{\Phi}_{13} + \dot{\Phi}_{33})^2 \right] \\ & + \frac{m_2}{4a^2} \left[\dot{U}_1^2 + \dot{U}_3^2 + \frac{a^2}{4} (\dot{\Phi}_{11} - \dot{\Phi}_{31})^2 + \frac{a^2}{4} (\dot{\Phi}_{13} - \dot{\Phi}_{33})^2 \right], \end{aligned} \quad (20)$$

where a dot represents the derivative with respect to time t .

To complete the continuum model, we derive the equations of motion and boundary conditions by the Hamilton's principle. Let A be a region of the thin film represented by the continuum model. Then the Hamilton's principle states

$$\delta \int_{t_0}^{t_1} \int_A (T - W) dV dt + \int_{t_0}^{t_1} \int_S (T_i \delta U_i + P_{ji} \delta \Phi_{ji}) dA dt = 0 \quad (21)$$

in which S is the entire boundary of A , T_i is external traction, and P_{ji} the external couple applied along S . Substituting Eqs. (15) and (20) in Eq. (21) and performing variations, we obtain the equations of motion:

$$\begin{aligned} -\frac{1}{2a^2} (m_1 + m_2) \ddot{U}_1 + \alpha_1 \left(2 \frac{\partial^2 U_1}{\partial X_1^2} - \frac{\partial \Phi_{11}}{\partial X_1} \right) \\ + \alpha_2 \left(2 \frac{\partial^2 U_1}{\partial X_1^2} + 2 \frac{\partial^2 U_1}{\partial X_3^2} + 2 \frac{\partial^2 U_3}{\partial X_1 \partial X_3} - \frac{\partial \Phi_{11}}{\partial X_1} - \frac{\partial \Phi_{31}}{\partial X_3} \right) = 0, \end{aligned} \quad (22)$$

$$\begin{aligned} -\frac{1}{2a^2} (m_1 + m_2) \ddot{U}_3 + \alpha_1 \left(2 \frac{\partial^2 U_3}{\partial X_1^2} - \frac{\partial \Phi_{33}}{\partial X_3} \right) \\ + \alpha_2 \left(2 \frac{\partial^2 U_3}{\partial X_1^2} + 2 \frac{\partial^2 U_3}{\partial X_3^2} + 2 \frac{\partial^2 U_1}{\partial X_1 \partial X_3} - \frac{\partial \Phi_{13}}{\partial X_1} - \frac{\partial \Phi_{33}}{\partial X_3} \right) = 0, \end{aligned} \quad (23)$$

$$\frac{1}{8} (m_1 + m_2) \ddot{\Phi}_{11} + \frac{1}{8} (m_1 - m_2) \ddot{\Phi}_{31} + (\alpha_1 + \alpha_2) \left(\Phi_{11} - \frac{\partial U_1}{\partial X_1} \right) = 0, \quad (24)$$

$$\frac{1}{8} (m_1 + m_2) \ddot{\Phi}_{33} + \frac{1}{8} (m_1 - m_2) \ddot{\Phi}_{13} + (\alpha_1 + \alpha_2) \left(\Phi_{33} - \frac{\partial U_3}{\partial X_3} \right) = 0, \quad (25)$$

$$\frac{1}{8} (m_1 + m_2) \ddot{\Phi}_{31} + \frac{1}{8} (m_1 - m_2) \ddot{\Phi}_{11} + \alpha_2 \left(\Phi_{31} - \frac{\partial U_1}{\partial X_3} \right) = 0, \quad (26)$$

$$\frac{1}{8} (m_1 + m_2) \ddot{\Phi}_{13} + \frac{1}{8} (m_1 - m_2) \ddot{\Phi}_{33} + \alpha_2 \left(\Phi_{13} - \frac{\partial U_3}{\partial X_1} \right) = 0. \quad (27)$$

The boundary conditions are

$$T_j = \left(\Sigma_{ji} + \sigma_{ji}^R \right) n_i, \quad P_{ji} = 0 \quad (28)$$

where n_i the unit vector normal to the boundary surface. It is noted that, for present continuum model developed based on the linear displacement expansion of Eq. (1), no couple stress is present.

The equations of motion for the reduced effective modulus theory are readily obtained by requiring $\gamma_{ij} = 0$ in the energy density function. We have

$$\alpha_1 \frac{\partial^2 U_1}{\partial X_1^2} + \alpha_2 \left(\frac{\partial^2 U_1}{\partial X_1^2} + \frac{\partial^2 U_1}{\partial X_3^2} + 2 \frac{\partial^2 U_3}{\partial X_1 \partial X_3} \right) = \frac{1}{2a^2} (m_1 + m_2) \ddot{U}_1, \quad (29)$$

$$\alpha_1 \frac{\partial^2 U_3}{\partial X_1^2} + \alpha_2 \left(\frac{\partial^2 U_3}{\partial X_1^2} + \frac{\partial^2 U_3}{\partial X_3^2} + 2 \frac{\partial^2 U_1}{\partial X_1 \partial X_3} \right) = \frac{1}{2a^2} (m_1 + m_2) \ddot{U}_3. \quad (30)$$

3. Wave propagation in thin film

The continuum theory with microstructures presented in Section 2 is now employed to study propagation of harmonic waves in a thin film of thickness h and of infinite in-plane dimensions. The thin film is assumed to consist of a number of atom layers, and the surfaces $X_3 = \pm \frac{h}{2}$ are free of tractions. Harmonic waves propagating in the X_1 -direction can be expressed as

$$U_1 = f_1(X_3) e^{ik(X_1 - ct)}, \quad U_3 = f_2(X_3) e^{ik(X_1 - ct)}, \quad (31)$$

$$\Phi_{11} = f_3(X_3) e^{ik(X_1 - ct)}, \quad \Phi_{33} = f_4(X_3) e^{ik(X_1 - ct)}, \quad (32)$$

$$\Phi_{31} = f_5(X_3) e^{ik(X_1 - ct)}, \quad \Phi_{13} = f_6(X_3) e^{ik(X_1 - ct)}, \quad (33)$$

where k denotes wave number, c is phase velocity, and $f_i(X_3)$ are unknown functions. Substituting Eqs. (31)–(33) in the equations of motion (22)–(27), we obtain

$$\left[\frac{(m_1 + m_2)\omega^2}{2a^2} - 2k^2(\alpha_1 + \alpha_2) \right] f_1 - ik(\alpha_1 + \alpha_2)f_3 + 2\alpha_1 f_1'' + 2ik\alpha_2 f_2' - \alpha_2 f_5' = 0, \quad (34)$$

$$\left[\frac{(m_1 + m_2)\omega^2}{2a^2} - 2k^2\alpha_2 \right] f_2 - ik\alpha_2 f_6 + 2(\alpha_1 + \alpha_2)f_2'' + 2ik\alpha_2 f_1' - \alpha_2 f_4' = 0, \quad (35)$$

$$-\frac{(m_1 + m_2)\omega^2}{8} f_3 - \frac{(m_1 - m_2)\omega^2}{8} f_5 + (\alpha_1 + \alpha_2)(f_3 - ikf_1) = 0, \quad (36)$$

$$-\frac{(m_1 + m_2)\omega^2}{8} f_4 - \frac{(m_1 - m_2)\omega^2}{8} f_6 + (\alpha_1 + \alpha_2)(f_2 - ikf_2') = 0, \quad (37)$$

$$-\frac{(m_1 + m_2)\omega^2}{8} f_5 - \frac{(m_1 - m_2)\omega^2}{8} f_3 + \alpha_2(f_5 - f_1') = 0, \quad (38)$$

$$-\frac{(m_1 + m_2)\omega^2}{8} f_6 - \frac{(m_1 - m_2)\omega^2}{8} f_4 + \alpha_2(f_6 - ikf_2) = 0, \quad (39)$$

where a prime indicates differentiation with respect to X_3 . By eliminating f_2, f_3, f_4, f_5 , and f_6 from Eqs. (34)–(39), the following differential equation for f_1 results:

$$C_1 C_5 f_1'''' + (C_5 C_2 + C_6 C_1) f_1''' - (C_4 C_8 - C_5 C_3 - C_6 C_2 - C_1 C_7) f_1'' + (C_3 C_6 + C_2 C_7) f_1' + C_7 C_3 f_1 = 0, \quad (40)$$

where

$$C_1 = (2 - D_8)\alpha_2, \quad C_2 = -ik(\alpha_1 + \alpha_2)D_2 - \alpha_2 D_7,$$

$$C_3 = \frac{\omega^2}{2a^2} (m_1 + m_2) - 2k^2(\alpha_1 + \alpha_2) - ik(\alpha_1 + \alpha_2)D_1,$$

$$C_4 = C_8 = 2ik\alpha_2, \quad C_5 = (\alpha_1 + \alpha_2)(2 - D_4),$$

$$C_6 = -(\alpha_1 + \alpha_2)D_3 - ik\alpha_2 D_6, \quad C_7 = \frac{\omega^2}{2a^2} (m_1 + m_2) - 2k^2\alpha_2 - ik\alpha_2 D_5,$$

$$D_1 = -ik(\alpha_1 + \alpha_2) \left[\frac{\omega^2}{2a^2} (m_1 + m_2) - \alpha_2 \right], \quad D_2 = \frac{\omega^2}{8a^2} (m_1 - m_2)\alpha_2,$$

$$\begin{aligned}
D_3 &= ik \frac{\omega^2}{8a^2} (m_1 - m_2) \alpha_2, & D_4 &= -(\alpha_1 + \alpha_2) \left[\frac{\omega^2}{2a^2} (m_1 + m_2) - \alpha_2 \right], \\
D_5 &= -ik \alpha_2 \left[\frac{\omega^2}{2a^2} (m_1 + m_2) - \alpha_1 - \alpha_2 \right], & D_6 &= \frac{\omega^2}{8a^2} (m_1 - m_2) (\alpha_1 + \alpha_2), \\
D_7 &= ik \frac{\omega^2}{8a^2} (m_1 - m_2) (\alpha_1 + \alpha_2), & D_8 &= -\alpha_2 \left[\frac{\omega^2}{2a^2} (m_1 + m_2) - \alpha_1 - \alpha_2 \right].
\end{aligned} \quad (41)$$

The general solutions of Eq. (40) for the function f_1 depend on the type of the roots of the characteristic equation

$$C_1 C_5 \beta^4 + (C_5 C_2 + C_6 C_1) \beta^3 - (C_4 C_8 - C_5 C_3 - C_6 C_2 - C_1 C_7) \beta^2 + (C_3 C_6 + C_2 C_7) \beta + C_7 C_3 = 0. \quad (42)$$

By solving the above biquadratic equation, the general solution for f_1 can be expressed as

$$f_1 = E_1 e^{\beta_1 X_3} + E_2 e^{\beta_2 X_3} + E_3 e^{\beta_3 X_3} + E_4 e^{\beta_4 X_3}, \quad (43)$$

where $\beta_1, \beta_2, \beta_3$, and β_4 are the four roots of Eq. (42). The solutions for other functions f_i , $i = 2-6$ can be obtained in a similar manner.

The traction-free boundary conditions at $X_3 = \pm \frac{h}{2}$ lead to

$$S_1 E_1 e^{(\beta_1 h/2)} + S_2 E_2 e^{(\beta_2 h/2)} + S_3 E_3 e^{(\beta_3 h/2)} + S_4 E_4 e^{(\beta_4 h/2)} = 0, \quad (44)$$

$$S_5 E_1 e^{(\beta_1 h/2)} + S_6 E_2 e^{(\beta_2 h/2)} + S_7 E_3 e^{(\beta_3 h/2)} + S_8 E_4 e^{(\beta_4 h/2)} = 0, \quad (45)$$

$$S_1 E_1 e^{(-\beta_1 h/2)} + S_2 E_2 e^{(-\beta_2 h/2)} + S_3 E_3 e^{(-\beta_3 h/2)} + S_4 E_4 e^{(-\beta_4 h/2)} = 0, \quad (46)$$

$$S_5 E_1 e^{(-\beta_1 h/2)} + S_6 E_2 e^{(-\beta_2 h/2)} + S_7 E_3 e^{(-\beta_3 h/2)} + S_8 E_4 e^{(-\beta_4 h/2)} = 0, \quad (47)$$

where

$$S_m = (2 - D_8) F_m + i k H_m - D_7, \quad S_{m+4} = (\alpha_1 + \alpha_2) [(2 - D_4) H_m - D_3 F_m] + i k \alpha_2,$$

$$F_m = \beta_m^3 \frac{C_5 C_1}{C_4 C_7} - \beta_m \frac{C_8 C_4 - C_5 C_3}{C_4 C_7}, \quad H_m = -\frac{1}{C_4} (C_3 + \beta_m^2 C_1), \quad m = 1, 2, 3, 4.$$

Eqs. (44)–(47) have nontrivial solutions for E_1, E_2, E_3 , and E_4 only if the determinant of the coefficients vanishes. This leads to the dispersion equation:

$$\begin{vmatrix}
S_1 e^{\beta_1 h/2} & S_2 e^{\beta_2 h/2} & S_3 e^{\beta_3 h/2} & S_4 e^{\beta_4 h/2} \\
S_5 e^{\beta_1 h/2} & S_6 e^{\beta_2 h/2} & S_7 e^{\beta_3 h/2} & S_8 e^{\beta_4 h/2} \\
S_1 e^{-\beta_1 h/2} & S_2 e^{-\beta_2 h/2} & S_3 e^{-\beta_3 h/2} & S_4 e^{-\beta_4 h/2} \\
S_5 e^{-\beta_1 h/2} & S_6 e^{-\beta_2 h/2} & S_7 e^{-\beta_3 h/2} & S_8 e^{-\beta_4 h/2}
\end{vmatrix} = 0. \quad (48)$$

4. Exact solution for wave propagation in lattice system

To validate the present continuum model, we now consider harmonic wave propagation in a two-dimensional lattice system as shown in Fig. 3. The lattice is assumed to be of infinite extent in the X_1 direction and the thickness in the X_3 -direction is h . The top and bottom layers are free surfaces.

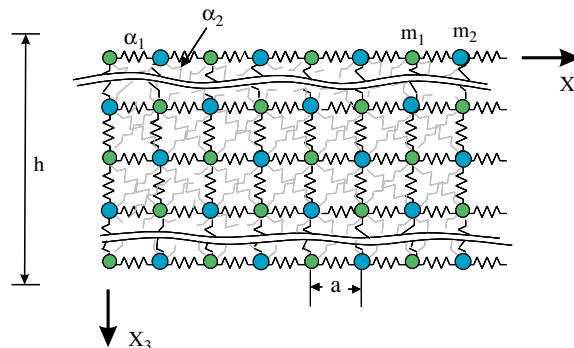


Fig. 3. The lattice system.

Along the thickness, the thin film is assumed to have N atom layers. The coordinate system is set up so that X_1 -axis coincides with the top layer of atoms and X_3 -axis coincides with an arbitrary column of atoms as shown in Fig. 3. Thus, the location of an arbitrary atom at $X_1 = ma$ and $X_3 = na$ can be denoted by $(X_1^{(m)}, X_3^{(n)})$. The displacements of this atom in X_1 - and X_3 -directions are denoted by $u_1^{(m,n)}$ and $u_3^{(m,n)}$, respectively.

Consider the i th column of atoms at $X_1 = ia$. The equations of motion for the atom at the top layer ($X_3 = 0$) is readily obtained as

$$m_1 \ddot{u}_1^{(i,0)} = -\alpha_1 (2u_1^{(i,0)} - u_1^{(i-1,0)} - u_1^{(i+1,0)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,1)} - u_1^{(i,0)} + u_3^{(i-1,1)} + u_3^{(i,0)}) \quad (49)$$

$$m_1 \ddot{u}_3^{(i,0)} = -\alpha_1 (u_3^{(i,0)} - u_3^{(i,1)}) + \frac{1}{2} \alpha_2 (-u_1^{(i+1,1)} + u_1^{(i,0)} + u_3^{(i+1,1)} - u_3^{(i,0)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,1)} - u_1^{(i,0)} + u_3^{(i-1,1)} - u_3^{(i,0)}) \quad (50)$$

in which the mass of the atom at the top layer is assumed to be m_1 . Similarly, the equations of motion for the atom at the bottom layer are

$$m_1 \ddot{u}_1^{(i,N)} = -\alpha_1 (2u_1^{(i,N)} - u_1^{(i-1,N)} - u_1^{(i+1,N)}) + \frac{1}{2} \alpha_2 (u_1^{(i+1,N-1)} - u_1^{(i,N)} + u_3^{(i+1,N-1)} - u_3^{(i,N-1)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,N-1)} - u_1^{(i,N)} - u_3^{(i-1,N-1)} + u_3^{(i,N)}), \quad (51)$$

$$m_1 \ddot{u}_3^{(i,N)} = -\alpha_1 (u_3^{(i,N)} - u_3^{(i,N-1)}) + \frac{1}{2} \alpha_2 (u_1^{(i+1,N-1)} - u_1^{(i,N)} + u_3^{(i+1,N-1)} - u_3^{(i,N)}) + \frac{1}{2} \alpha_2 (-u_1^{(i-1,N-1)} + u_1^{(i,N)} + u_3^{(i-1,N-1)} - u_3^{(i,N)}), \quad (52)$$

where the mass of the atom at the bottom layer is also assumed to be m_1 in order to make the lattice system symmetric with respect to its mid-plane.

The equations of motion for the interior atoms in the i th column are

$$m \ddot{u}_1^{(i,j)} = -\alpha_1 (2u_1^{(i,j)} - u_1^{(i-1,j)} - u_1^{(i+1,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i+1,j+1)} - u_1^{(i,j)} + u_3^{(i+1,j+1)} - u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i+1,j-1)} - u_1^{(i,j)} - u_3^{(i+1,j-1)} + u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,j-1)} - u_1^{(i,j)} + u_3^{(i-1,j-1)} - u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,j+1)} - u_1^{(i,j)} - u_3^{(i-1,j+1)} + u_3^{(i,j)}), \quad (53)$$

$$m \ddot{u}_3^{(i,j)} = -\alpha_1 (2u_3^{(i,j)} - u_3^{(i-1,j)} - u_3^{(i+1,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i+1,j+1)} - u_1^{(i,j)} + u_3^{(i+1,j+1)} - u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (-u_1^{(i+1,j-1)} + u_1^{(i,j)} + u_3^{(i+1,j-1)} - u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (u_1^{(i-1,j-1)} - u_1^{(i,j)} + u_3^{(i-1,j-1)} - u_3^{(i,j)}) + \frac{1}{2} \alpha_2 (-u_1^{(i-1,j+1)} + u_1^{(i,j)} + u_3^{(i-1,j+1)} - u_3^{(i,j)}), \quad (54)$$

where $j = 1, 2, 3, \dots, N-1$ and $m = m_1$ if j is an even number and $m = m_2$ otherwise.

For a plane harmonic wave propagating in the X_1 -direction, the displacements can be assumed as

$$u_1^{(l,n)} = B_1^n e^{ik(X_1^l - ct)}, \quad u_3^{(l,n)} = B_3^n e^{ik(X_1^l - ct)}, \quad (55)$$

where k denotes wave number, c is phase velocity, and $X_1^l = la$. Substitution of Eq. (55) in Eqs. (39)–(54) yields $2N$ equations for the unknown coefficient vector $B = \{B_1^1, B_3^1, \dots, B_1^j, B_3^j, \dots, B_1^N, B_3^N\}$. The dispersion equation is obtained by requiring that the determinant of the coefficient matrix vanishes.

Figs. 4 and 5 show the comparison of dispersion curves for the lowest symmetric mode and anti-symmetric mode obtained according to Eq. (48) of the continuum model with microstructures, the effective modulus theory (29) and (30), and the exact solution for the lattice system, respectively. The parameters used in the calculation for the cubic crystal structure are $a = 1.74 \times 10^{-10}$ m, $\alpha_1 = 2.02$ N/m, $\alpha_2 = 1.10$ N/m, $m_2/m_1 = 10$ and the film thickness is $h = 8a$ (i.e., 7 atom layers). The normalized wave velocity $c^* = c/\sqrt{\frac{2\gamma}{\rho_0}}$, with $\rho_0 = \frac{m_1+m_2}{2a^2}$, is used in the figure. The results of Fig. 4 clearly show that both the effective modulus theory and the continuum model

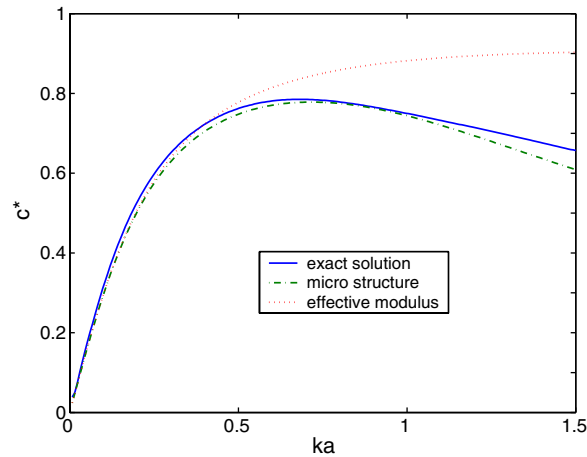


Fig. 4. Dispersive curves for antisymmetric mode obtained with the lattice model and continuum models for a thin film with 7 atom layers.

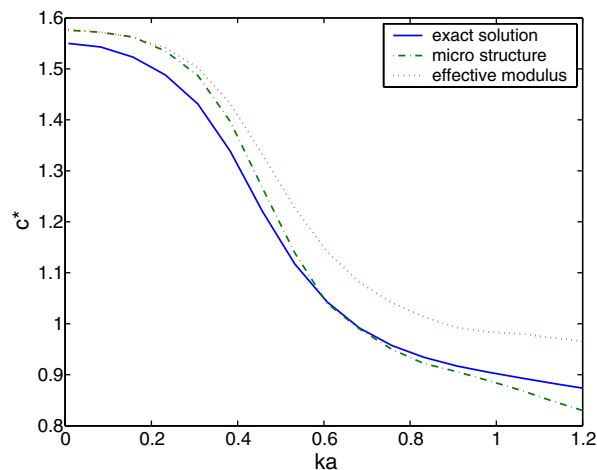


Fig. 5. Dispersive curves for symmetric mode obtained with the lattice model and the continuum models for a thin film consisting of 7 atom layers.

with microstructures yield very good predictions for the anti-symmetric wave for long waves with $ka < 0.5$. This is expected because at lower frequencies wave dispersion is mainly caused by the finite thickness of the film and not by the effect of microstructures. However, as wave length decreases, the dispersion curve computed from the effective modulus theory deviates substantially from the exact curve, while the curve predicted by the continuum theory with microstructures is in good agreement with the exact curve. On the other hand if one employs the effective modulus theory and waves with $ka > 0.5$ to determine elastic constants of a thin film with the aid of the dispersion relations, the values of these constants may be significantly overestimated.

Fig. 5 shows the dispersion curves for the lowest symmetric mode. The dispersion curve predicted by the present continuum model with microstructures shows a better agreement with the exact solution than that by the effective modulus theory. It is of interest to note that the results by both continuum theories show some difference relative to the exact phase velocity at long wave lengths. This discrepancy is attributed to the fact both the present continuum theory and the effective modulus theory are not capable of accounting for the nanoscale surface effect on the thin film. However, this surface effect can be neglected in thin films consisting of 20 or more atom layers (Sun and Zhang, 2003) which amount to 6–7 nm. Consequently, if one wants to use the lowest symmetric wave mode to determined thin film material properties, some data corrections should be exercised when the thickness of thin film is less than 6–7 nm.

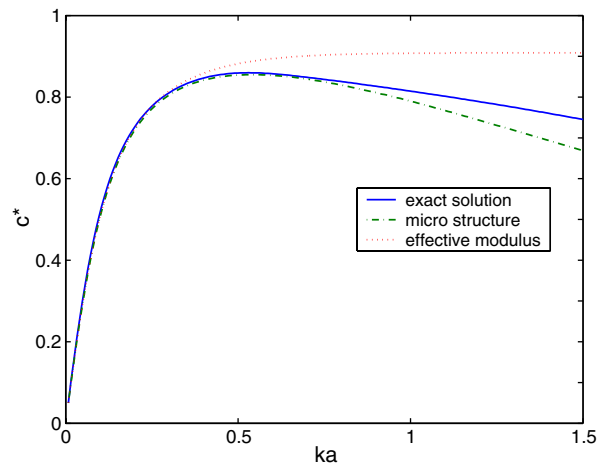


Fig. 6. Dispersive curves for antisymmetric mode obtained with the lattice model and the microstructure continuum model for a thin film consisting of 45 atom layers.

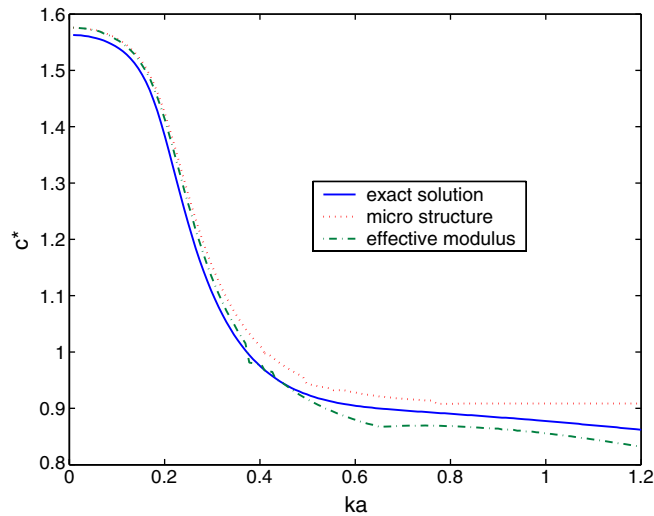


Fig. 7. Dispersive curves for the symmetric mode obtained with the lattice model and the continuum models for a thin film consisting of 45 atom layers.

Figs. 6 and 7 show comparisons of dispersion curves for thin films of thickness $h = 15a$. Conclusions similar to those for the results of Figs. 4 and 5 can be made here except for phase velocities at long wave lengths, which are found to be in fairly good agreement with that of the exact lattice model.

5. Surface wave propagation

This section concerns surface wave propagation in the two-dimensional lattice system. It is well known that in a classical elastic solid, the Rayleigh surface wave is nondispersive. However, surface waves with wavelengths that are comparable to the atomic spacing must be carefully examined if the surface wave technique is to be used in measuring material constants. It is noteworthy that, especially in electronic device applications, surface wave frequencies on the order of GHz–THz are now possible for this type of measurement.

We now consider the two-dimensional problem of waves propagating along the surface of a semi-infinite continuum with microstructure as schematically shown in Fig. 8. This continuum is assumed to represent a

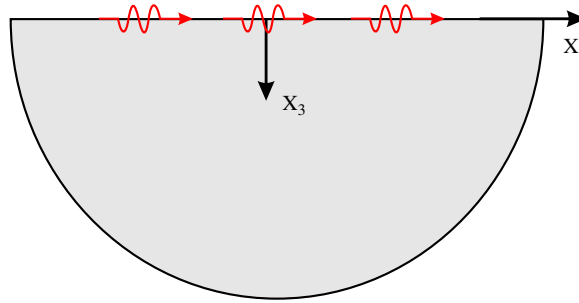


Fig. 8. Surface wave propagation in the generalized elastic medium.

material of the cubic structure and X_1 -axis is parallel to the $[100]$ crystal direction. The general solution given in Section 3 for plate-like thin films is still valid except for the boundary conditions which are now given by

$$T_j = (\Sigma_{ji} + \sigma_{ji}^R)n_i = 0, \quad i, j = 1, 3 \text{ at } X_3 = 0, \quad (56)$$

$$U_j = 0, \quad j = 1, 3 \text{ as } X_j \rightarrow \infty. \quad (57)$$

The conditions of Eq. (57) require that only the two roots of β of Eq. (41) with negative real parts are permissible solutions for the surface wave problem. Denoting these two roots by β_1 and β_2 , we write the solution for f_1 as

$$f_1 = E_1 e^{(\beta_1 X_3)} + E_2 e^{(\beta_2 X_3)}. \quad (58)$$

The corresponding functions f_2, f_3, f_4, f_5 , and f_6 can be obtained by solving Eqs. (32)–(39) with f_1 treated as a known function. Finally, the traction free surface condition (56) yields

$$S_1 E_1 + S_2 E_2 = 0, \quad (59)$$

$$S_5 E_1 + S_6 E_2 = 0, \quad (60)$$

where

$$\begin{aligned} S_1 &= (2 - D_8)F_1 + ikH_1 - D_7, & S_2 &= (2 - D_8)F_2 + ikH_2 - D_7, \\ S_5 &= (\alpha_1 + \alpha_2)[(2 - D_4)H_1 - D_3F_1] + ik\alpha_2, & S_6 &= (\alpha_1 + \alpha_2)[(2 - D_4)H_2 - D_3F_2] + ik\alpha_2, \\ F_1 &= \beta_1^3 \frac{C_5 C_1}{C_4 C_7} - \beta_1 \frac{C_8 C_4 - C_5 C_3}{C_4 C_7}, & F_2 &= \beta_2^3 \frac{C_5 C_1}{C_4 C_7} - \beta_2 \frac{C_8 C_4 - C_5 C_3}{C_4 C_7}, \\ H_1 &= -\frac{1}{C_4}(C_3 + \beta_1^2 C_1), & H_2 &= -\frac{1}{C_4}(C_3 + \beta_2^2 C_1). \end{aligned}$$

As usual, the homogeneous system of Eqs. (59) and (60) yield the Rayleigh wave equation:

$$\frac{(2 - D_8)F_1 - D_7 + ikH_1}{(\alpha_1 + \alpha_2)[(2 - D_4)H_1 - D_3F_1] + ik\alpha_2} = -\frac{(2 - D_8)F_2 - D_7 + ikH_2}{(\alpha_1 + \alpha_2)[(2 - D_4)H_2 - D_3F_2] + ik\alpha_2}. \quad (61)$$

The exact solution for surface waves in a half-space lattice is also obtained by using the governing Eqs. (49), (50) and (53), (54) for the lattice system. To simulate the semi-infinite medium, lattice systems of 90 and 110 layers of atoms are both used with the bottom layer fixed. The results indicate that there is little difference between the two solutions.

Fig. 9 shows the dispersion curves for surface waves obtained according to Eq. (61), effective modulus theory, and the corresponding lattice system, respectively. The parameters of the cubic crystal structure used in the calculations are $a = 1.74 \times 10^{-10}$ m, $\alpha_1 = 2.02$ N/m, $\alpha_2 = 1.10$ N/m, $m_2/m_1 = 10$. For this set of material parameters, the roots are $\beta_1 = -4.2 \times 10^7 + 1.01 \times 10^7 i$ and $\beta_2 = -4.2 \times 10^7 - 1.01 \times 10^7 i$ for $ka = 0.015$. The resulting displacement components in the X_3 -direction are found to decay rapidly along the X_3 -axis. The rate of decay depends on wave length. In general, the displacement components diminish within about two times the wave length. From Fig. 9, it is evident that, unlike the classical continuum, surface waves in the lattice system are

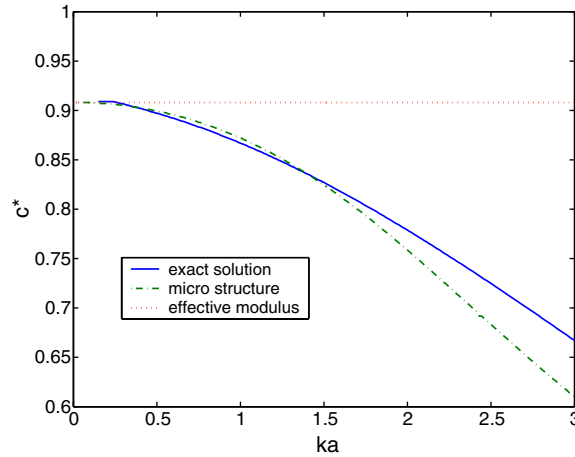


Fig. 9. Dispersive curves for surface waves obtained with the lattice model, the continuum theory with microstructures, and the effective modulus theory.

dispersive and the present continuum model with microstructures describes this dispersive behavior pretty well. In contrast, the effective modulus theory fails to capture it.

6. Surface wave propagation in thin film on an elastic substrate

Thin films are often supported by a thicker substrate as shown in Fig. 10. The Lamé constants of the substrate are denoted by λ and μ . The longitudinal and transverse shear wave velocities of the substrate are $\bar{c}_L = \sqrt{\frac{\lambda+2\mu}{\rho}}$ and $\bar{c}_T = \sqrt{\frac{\mu}{\rho}}$, respectively, and ρ is mass density.

To study wave propagation in this layered system, we use the continuum model with microstructures to represent the thin film. The substrate is a classical elastic solid for which the general form of the solution for harmonic waves is readily obtained. For simplicity, the wave propagation term $e^{ik(X_1-ct)}$ is dropped and the amplitudes of displacement components and stress components in the substrate are given by

$$U_1^s = ikB_1^s e^{-k\bar{\alpha}X_3} - B_2^s \bar{\beta} e^{-k\bar{\beta}X_3}, \quad (62)$$

$$U_3^s = -(B_1^s \bar{\alpha} e^{-k\bar{\alpha}X_3} + ikB_2^s e^{-k\bar{\beta}X_3}), \quad (63)$$

$$\Sigma_{33}^s = \mu k^2 [(1 + \bar{\beta}^2) B_1^s e^{-k\bar{\alpha}X_3} + 2iB_2^s \bar{\beta} e^{-k\bar{\beta}X_3}], \quad (64)$$

$$\Sigma_{31}^s = \mu k^2 [-2iB_1^s \bar{\alpha} e^{-k\bar{\alpha}X_3} + B_2^s (1 + \bar{\beta}^2) e^{-k\bar{\beta}X_3}], \quad (65)$$

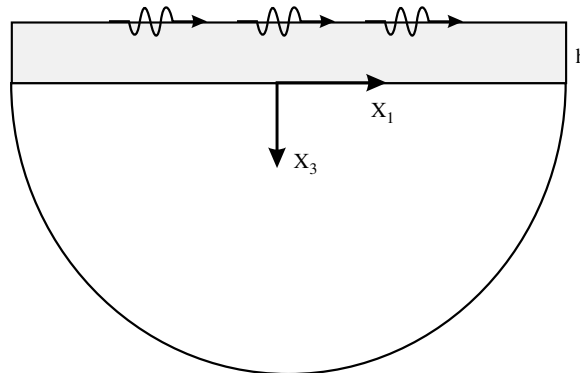


Fig. 10. Surface wave in the thin film bonded to the elastic medium.

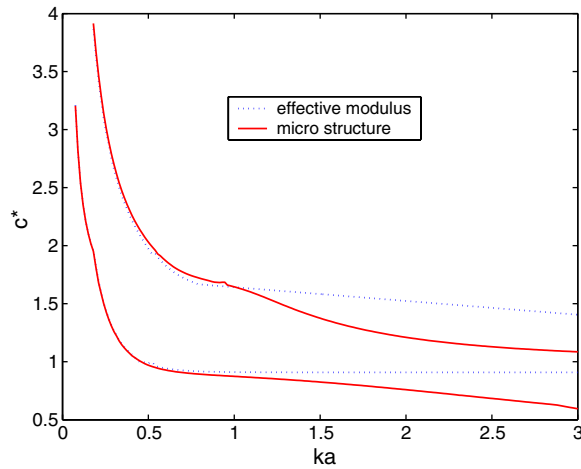


Fig. 11. Dispersive curves obtained using the continuum model with microstructures and the effective modulus theory.

where superscript “s” denotes substrate, $\bar{\alpha} = \sqrt{1 - \frac{c_s^2}{c_L^2}}$, $\bar{\beta} = \sqrt{1 - \frac{c_s^2}{c_T^2}}$, and B_1^s and B_2^s are unknown coefficients to be determined.

For the thin film represented by the continuum with microstructures, the general solution presented in Section 3 is valid for the present case. This solution and the solution for the substrate must satisfy the free surface boundary and interlayer continuity conditions, i.e.,

$$T_j = (\Sigma_{ji} + \sigma_{ji}^R)n_i = 0 \quad \text{at } X_3 = -h, \quad (66)$$

$$U_j = U_j^s, \quad T_j = T_j^s \quad \text{at } X_3 = 0 \quad (67)$$

in addition to the finiteness condition

$$U_j^s = 0 \quad \text{as } X_j \rightarrow \infty. \quad (68)$$

Conditions (66) and (67) result in the dispersion equation:

$$\begin{vmatrix} S_1 e^{(-\beta_1 h)} & S_2 e^{(-\beta_2 h)} & S_3 e^{(-\beta_3 h)} & S_4 e^{(-\beta_4 h)} & 0 & 0 \\ S_5 e^{(-\beta_1 h)} & S_6 e^{(-\beta_2 h)} & S_7 e^{(-\beta_3 h)} & S_8 e^{(-\beta_4 h)} & 0 & 0 \\ 1 & 1 & 1 & 1 & ik & -\bar{\beta} \\ F_1 & F_2 & F_3 & F_4 & -\bar{\alpha} & ik \\ S_1 & S_2 & S_3 & S_4 & \mu k^2(1 + \bar{\beta}^2) & 2i\mu k^2 \bar{\beta} \\ S_5 & S_6 & S_7 & S_8 & 2i\mu k^2 \bar{\alpha} & \mu k^2(1 + \bar{\beta}^2) \end{vmatrix} = 0. \quad (69)$$

Fig. 11 shows the comparison of the dispersion curves for the first two lowest modes. The parameters used in the calculation for the cubic crystal structure for the thin film are $a = 1.74 \times 10^{-10}$ m, $\alpha_1 = 2.02$ N/m, $\alpha_2 = 1.10$ N/m, $m_2/m_1 = 10$ and $h/a = 15$. The Lamé constants of the elastic substrate are $\lambda = 6.05 \times 10^{10}$ Pa, $\mu = 2.59 \times 10^{10}$ Pa, and $\nu = 0.35$, $\rho = 2700$ kg/m³. The dashed lines represent the results of the effective modulus theory, and solid lines indicate the results of the continuum theory with microstructures. It is evident that for the long waves, both continuum theories give good predictions for phase velocity. However, for shorter waves ($ka > 0.5$), the dispersion curves from these two continuum theories are substantially different. From the displacement profile for waves of longer wavelengths, it is seen that the participation of the substrate is significant, while for waves of shorter wavelengths, say $ka > 0.5$, the deformation involves predominantly the thin film. Thus, using the surface wave technique to determine the thin film properties, waves of shorter wavelengths seem to be more desirable.

7. Concluding remarks

In this paper, we have examined the validity in using the classical continuum (effective modulus) theory and a continuum theory with microstructures to analyze high frequency/short wavelength harmonic waves in thin films. It was found that the effective modulus theory is inadequate for describing waves of short wavelengths propagating in thin films. It was also found that the continuum theory with microstructures provides much more accurate predictions of dispersive wave velocities for surface waves of short wavelengths which can be used to determine elastic constants of thin films.

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