Examining and calculation of non-classical in the solutions to the true elastic cable under concentrated loads in nanofilm

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ABSTRACT: Due to high surface-to-volume ratio of nanoscale structures, surface stress effects have a significant influence on their behavior. In this paper, a two-dimensional problem for an elastic layer that is bonded to a rigid substrate and subjected to an inclined concentrated line load acting on the surface of the layer is investigated based on Gurtin-Murdoch continuum model to consider surface stress effects. Fourier integral transforms are used to solve the non-classical boundary-value problem related to inclined point load and an analytical solution is obtained for the corresponding boundary-value problem. Selected numerical results are presented for different values of loading angle and are compared with the classical ones to illustrate the influence of the surface stress effects on the stiffness of nano-coating and ultra-thin films. It is found that the surface stress effects have a quite large influence on the response of the nanofilm especially for more vertical loading (higher values of the angle of loading) and make the layer stiffer than the classical case.

Keywords: Boundary-value problem; Elasticity; Nanomechanics; Point loading; Surface stress.

INTRODUCTION

Nanoscience and nanotechnology have generated considerable interest and have attracted much investment in order to develop new revolutionary applications in a wide range of disciplines. To successfully design and manufacture the nanostructures and systems, a fundamental study of their mechanical behavior is essential. Nanomechanics are the area of mechanics in which the mechanical properties and behavior of materials and structures at the nanoscale are studied.

An interesting class of problems in nanoscale mechanics deals with exceptional response and properties due to surface energy effects. These effects can be more substantial especially for thin films where there are a great number of atoms near the surface in comparison with that in the bulk. Thin films have many applications such as corrosion resistant coating, microelectronics and integrated circuits, etc. Vinci and Vlassak [1] reviewed the mechanical behavior of thin films, and proposed new experimental techniques to measure thin film properties. Zhao et al. [2] introduced a method that utilizes only the loading curves of an indentation test to extract the elastoplastic properties of an elastic-perfectly plastic thin film as well as the plastic properties of a work hardening thin film. Pervan et al. [3] studied the growth mode, structural and electronic properties of ultra-thin films at room temperature by means of Auger electron spectroscopy, low energy electron diffraction and angular-resolved photoemission. Ngo et al. [4] investigated the stress field in a multilayer thin films-substrate system subjected to non-uniform temperature and misfit strains based on an extension of the classical Stoney formula.

Contact mechanics problem of a surface-loaded layer based on a rigid base has a wide range of practical applications in the field of microelectronics, nano-indentation, and surface coating. Chen et al. [5] studied the mechanical properties of thin film-substrate systems by nano-indentation, considering the effects of thickness and different coating-substrate
combinations. They found that the classical plasticity theory cannot predict the experimental results, even considering the indenter tip curvature. Li et al. [6] investigated the influence of contact geometry, including the round tip of the indenter and the roughness of the specimen, on hardness behavior for elastic-plastic materials by means of finite element simulation. Dhaliwal and Rau [7,8] reduced the axisymmetric Boussinesq problem of an elastic layer lying over an elastic half-space to a Fredholm integral equation that was solved numerically to obtain the elastic field.

Nowadays, a film can be made as thin as few nanometers using modern processing technologies. Yasumoto and Tomimasu [9] proposed a novel method for thin film fabrication using the mid-infrared free electron laser having a tunable wavelength. Iitaka et al. [10] demonstrated combinatorial approach in investigation of organic thin film fabrication. Through high ratio of surface to volume of ultra-thin films, it is necessary to consider surface stress effects, which is usually neglected in the classical mechanics. Gurtin and Murdoch [11,12] proposed a generic theoretical approach based on continuum mechanics concepts to account the surface energy. The Gurtin-Murdoch surface stress model has recently been used to consider surface stress effects in modern contact problems. Mogilevskaya et al. [13] analyzed a two-dimensional problem of multiple interacting circular nano-inhomogeneities based on the Gurtin-Murdoch model. Li et al. [14] examined the effect of surface stress on stress concentration near a spherical void in an elastic medium using Gurtin-Murdoch continuum elasticity. He and Lim [15] derived surface Green function for incompressible, elastically isotropic half-space coupled with surface stress by using double Fourier transform technique and Gurtin-Murdoch model. Gordeliy et al. [16] used the generalized Gurtin-Murdoch model for a two-dimensional, transient, uncoupled thermoelastic problem of an infinite medium with a circular nano-scale cavity. Based on the surface elasticity theory, Koguchi [17] presented Green’s functions for anisotropic elastic half-space using Stroh’s formulas. Bar On et al. [18] developed a continuum model for nanobeams, including both surface effects and material heterogeneity. A comparison between continuum and atomistic solutions revealed differences. This result, originated from local transition effects in the neighborhood of strong non-uniformities. Shen and Hu [19] proposed an elastic enthalpy variational principle for nanosized dielectrics concerning with the flexoelectric effect, the surface effects and the electrostatic force where surface effects contain the effects of both surface stress and surface polarization.

According to the above literature review, it can be concluded that developed solutions based on Gurtin-Murdoch continuum elasticity accounting for the surface stress effects is necessary to study nanofilms. In this work, a general two-dimensional problem for an isotropic elastic ultra-thin film bonded to a rigid substrate and subjected to incline concentrated loading is considered in the presence of surface stress effects.

**EXPERIMENTAL**

**Fundamental Equations**

The constitutive relations of the bulk material relating non-zero stresses to the corresponding strains can be expressed as

\[
\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\delta_{ij}\varepsilon_{kk}
\]

where \(\sigma_{ij}\) and \(\varepsilon_{ij}\) denote, in sequence, components of displacement and stress, \(\delta_{ij}\) is the usual Kronecker delta, \(\mu\) and \(\lambda\) are the Lame constants of the bulk material.

According to the Gurtin-Murdoch continuum model, surface constitutive relation can be obtained as

\[
\sigma_{ij}^0 = \tau_0\delta_{ij} + (\lambda_0 + \tau_0)\varepsilon_{ii} + 2(\mu_0 - \tau_0)\varepsilon_{ij}
\]

where \(\tau_0\) is the surface residual stress without constraint; \(\lambda_0\) and \(\mu_0\) are surface Lame constants or surface elastic constants.

Note that the surface stress is a second rank tensor in tangent plane of the surface, so \(\alpha\) and \(\beta\) take integers 1 or 2.

**Non-Classical Solution for Displacement and Stress Components**

**Non-Classical Solution with Finite Thickness of Layer:**

The nanofilm considered herein is an elastic layer with finite thickness subjected to external inclined point loading on the surface. A Cartesian coordinate system \((x_1, x_2, x_3)\) is introduced as shown in Fig. 1.
The displacement and stress components are indicated by $u_{i}$ and $\varphi_{i}$, respectively. The general solution for these components of displacement and stress for a two-dimensional elastic layer can be expressed using Fourier integral transforms as [20,21]

\[ u_1 = \frac{1}{4\pi\mu} \int_{-\infty}^{\infty} \left\{ \left[ A\eta - B \left( \frac{\lambda + 2\mu}{\lambda + \mu} \eta - x_3 \eta \right) \right] e^{-x_3 \eta} \right\} e^{-ix_3 \eta} d\eta + \left[ C\eta + D \left( \frac{\lambda + 2\mu}{\lambda + \mu} + x_3 \eta \right) \right] e^{x_3 \eta} \right\} e^{-ix_3 \eta} d\eta \]

\[ u_3 = \frac{1}{4\pi\mu} \int_{-\infty}^{\infty} \left\{ \left[ A\eta + B \left( \frac{\lambda + 2\mu}{\lambda + \mu} + x_3 \eta \right) \right] e^{-x_3 \eta} \right\} e^{-ix_3 \eta} d\eta + \left[ -C\eta + D \left( \frac{\lambda + 2\mu}{\lambda + \mu} - x_3 \eta \right) \right] e^{x_3 \eta} \right\} e^{-ix_3 \eta} d\eta \]

\[ \sigma_{11} = \frac{1}{2\pi} \int_{0}^{2\pi} \left\{ \left[ (A\eta^2 - B(2\eta^2 + x_2^2)) e^{-x_3 \eta} \right] + \right] \left[ C\eta^2 + D(2\eta^2 + x_3^2) e^{x_3 \eta} \right] \right\} e^{-ix_3 \eta} d\eta \]

\[ \sigma_{33} = \frac{1}{2\pi} \int_{0}^{2\pi} \eta \left\{ \left[ A\eta^2 + B(1 - x_2^2) e^{-x_3 \eta} \right] + \right] \left[ C\eta^2 + D(1 + x_3^2) e^{x_3 \eta} \right] \right\} e^{-ix_3 \eta} d\eta \]

By applying Fourier integral transform to equations (4) and substituting equation (3), the following equations can be obtained:

\[ A + C = \frac{2\lambda}{\eta} \]

\[ B + D - (A - C)\eta - \frac{2\mu + \lambda}{2\mu} \left[ \left( \frac{\lambda + 2\mu}{\lambda + \mu} \right) D + B \right] \eta + (A + C)\eta = \frac{P_t}{\eta} \]

\[ \left[ \frac{\mu}{\lambda + \mu} B + (A + Bh)\eta \right] e^{-h\|\eta\|} + \left[ \frac{\mu}{\lambda + \mu} - D + (C + Dh)\eta \right] e^{h\|\eta\|} = 0 \]

\[ \left[ \frac{\lambda + 2\mu}{\lambda + \mu} B + (A + Bh)\eta \right] e^{-h\|\eta\|} + \left[ \frac{\lambda + 2\mu}{\lambda + \mu} - D + (C + Dh)\eta \right] e^{h\|\eta\|} = 0 \]

where $P_t$ and $P_e$ are the Fourier integral transforms of $p_t(x_1)$ and $p_e(x_1)$, respectively.

The coefficients $A, B, C$ and $D$ can be obtained by solving the equations (5) as

\[ A = \frac{A^1 + iA^2}{H} , \quad B = \frac{B + iB^2}{H} , \quad C = \frac{C + iC^2}{H} , \quad D = \frac{D + iD^2}{H} \]

\[ A^1 = \frac{P_t}{2\eta^2} \left( \left( \lambda + 3\mu \right) \left( 1 + \psi \eta |\eta| \right) e^{2h|\eta|} - \psi |\eta| \right) + 2h\eta^2 (\lambda + \mu) (\eta + h) - \frac{2(\lambda + 2\mu)^2}{\lambda + 2\mu} \psi h^2 |\eta|^3 \]

\[ A^2 = -\frac{P_t}{|\eta|\eta} \left[ \frac{\mu(\lambda + 2\mu)}{\lambda + \mu} + (\lambda + \mu) h^2 |\eta|^2 \right] \]

\[ A^3 = \frac{P_t}{|\eta|\eta} \left[ \frac{\mu(\lambda + 2\mu)}{\lambda + \mu} + (\lambda + \mu) h^2 |\eta|^2 \right] \]
If \( \psi = 0 \), the solution obviously reduces to the classical elasticity solution.

Non-Classical Solution with Infinite Thickness of Layer

When the value of thickness of a nanofilm is so larger than its other dimensions, it can be assumed that \( h \) approaches infinity, and the above solution will be reduced to the following closed-form

\[
\begin{align*}
B' &= \frac{P_0}{2\eta} \left[ (\lambda + 3\mu) \left[ 1 + \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] - \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] \\
B'' &= \frac{P_0}{2\eta} \left[ (\lambda + 3\mu) \left[ 1 + \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] + (\lambda + \mu) (1 + 2h \eta) \right] \\
C' &= \frac{P_0}{2\eta^2} \left[ (\lambda + 3\mu) \left[ 1 - \psi \eta^2 \right] - \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] + 2\eta h \left[ (\lambda + \mu) \psi + h \right] + \frac{\lambda^2 + 4\lambda \mu + 5\mu^2}{\lambda + \mu} \\
C'' &= \frac{P_0}{\eta^2} \left[ \frac{\mu(\lambda + 2\mu)}{\lambda + \mu} + (\lambda + \mu) h \eta^2 \right] \\
D' &= \frac{P_0}{2\eta} \left[ (\lambda + 3\mu) \left[ 1 - \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] + \frac{\lambda + \mu}{\lambda + 2\mu} \psi \eta^2 \right] + 2\eta h \left[ (\lambda + \mu) \psi + h \right] + \frac{\lambda^2 + 4\lambda \mu + 5\mu^2}{\lambda + \mu} \\
D'' &= \frac{P_0}{2\eta} \left[ (\lambda + 3\mu) \left[ 1 - \psi \eta^2 \right] + (\lambda + \mu) (1 + 2h \eta) \right] \\
H &= (\lambda + 3\mu) \left[ \cosh(2\eta h) \right] + \psi \eta \sinh(2\eta h) + 2\eta h \left[ (\lambda + \mu) \psi + h \right] + \frac{\lambda^2 + 4\lambda \mu + 5\mu^2}{\lambda + \mu}
\end{align*}
\]

and \( \psi = \frac{2(\mu + \lambda h^2)}{\lambda + \mu} \) is a constant with the dimension of length. In the absence of surface stress effects, the value of \( \psi \) will be vanished and the solution will be reduced to the classical one.

RESULTS AND DISCUSSION

Numerical Results

As it was shown in the previous sections, a closed-form solution for the case of a nanofilm with finite value of thickness cannot be obtained due to the complexity of the integrants. However, numerical technique is used to calculate the elastic field of a layer with finite thickness. In this section, selected numerical results are presented for Nickel [1 1 1] surface to indicate the influence of surface stress effects on the elastic field of ultra-thin layer subjected to inclined point loading. The material surface constants corresponding to Nickel surface can be obtained from atomistic simulations [22, 23], which are: \( \mu_0 = 1.655 \, N/m, \lambda_0 = 1.247 \, N/m, \tau_0 = 0.1154 \, N/m \). The bulk elastic
constants for Nickel are: $\mu = 76 \text{ GPa}$, $\lambda = 126.2 \text{ GPa}$ [24]. In the following numerical results for the case of finite thickness of layer, it is taken that $h = 40\psi$. The non-dimensional coordinates are used to show the numerical results as: $\bar{x}_1 = x_1/\psi$, $\bar{x}_2 = x_2/\psi$, $\bar{h} = h/\psi$.

Depicted in Figs. 2 and 3 are the distributions of the surface displacements of the nanofilm due to inclined point loading with angle of $\alpha = 45^\circ$ at different depths of the layer. It can be seen that the surface stress effects have significant influence on the distribution of displacement especially at lower depth of the layer and make the layer stiffer than the classical case. However, both in classical and non-classical solutions displacements decrease at lower depth of the layer.

Figs. 4-6 show the stress profiles of the nanofilm at different depths of the layer under inclined point load with angle of $\alpha$. The remarkable influence of surface stress effects on the distribution of stress is found clearly. Also, the stiffening behavior through surface stress effects observed previously for displacement profiles can be seen for the distribution of stresses in all cases of depth of the layer.

Figs. 7-11 illustrate the influence of angle of loading on the distribution of different components of displacement and stress along the $x_1$ axis. It is found that with increase of angle of loading (approaching to vertical point load) surface stress effects are more important and stiffening the layer due to these effects is quiet significant for upper values of $\alpha$. So, it can be concluded that the surface stress effects have more remarkable influence on the displacement and stress profiles for the case of vertical point load in comparison with the horizontal point load.
Fig. 4: Distribution of nondimensional horizontal stress at different depths of the layer.

Fig. 5: Distribution of nondimensional vertical stress at different depths of the layer along the axis.

Fig. 6: Distribution of nondimensional shear stress at different depths of the layer along the axis.
Fig. 7: Variation of nondimensional horizontal displacement profile versus the angle of loading along the axis.

Fig. 8: Variation of nondimensional vertical displacement profile versus the angle of loading along the axis.

Fig. 9: Variation of nondimensional horizontal stress profile versus the angle of loading along the $x_2$ axis ($x_2 = 0.3$).
Fig. 10: Variation of nondimensional vertical stress profile versus the angle of loading along the $x_1$ axis ($\xi_1 = 0.3$).

Fig. 11: Variation of nondimensional shear stress profile versus the angle of loading along the $x_2$ axis ($\xi_2 = 0.3$).

**Convergence of the numerical results**

In Tables 1 and 2, the convergence criterion of some of the selected numerical results is examined. It is observed from these tables that the convergence is achieved rapidly.

In Table 1, the value of non-dimensional displacement components are given for the layer with different thicknesses and $\xi_1 = 0.5$. Table 2 shows the values of non-dimensional stress components at different depths of the layer with the layer thickness $h = 40 \psi$ and $\gamma$. The Gauss quadrature technique is used to calculate numerical integration. In each iteration, the number of intervals has increased from the previous one to decrease the error of approximation. This pattern of convergence of the numerical technique reflects its efficiency and accuracy.
CONCLUSION

This work presents a non-classical continuum model accounting for surface stress effects based on Gurtin-Murdoch elasticity theory to analyze the elastic field of nanofilms subjected to inclined point load. The analysis is performed assuming both finite and infinite thickness of layer. Selected numerical results are presented to demonstrate the salient features of the response of the layer to assess the influence of surface stress effects. The governing equations are developed for inclined point load with arbitrary value of angle of loading. It is shown that close form analytical solution can be obtained for the case of infinite thickness of the layer. The present non-classical solution shows that the surface elastic properties make the material stiffer than the classical case through consideration of surface stress effects.

It is found that in the lower depths of the layer, the surface stress effects have more significant influence on the displacement and stress profiles and have little influence on the base of the layer. Also, it is shown that by approaching the case of vertical point load (by increasing the value of $\alpha$), the influence of surface stress effects is quiet strong compared to horizontal point loading.

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