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Finite element analysis of functionally graded nano-scale films

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ABSTRACT

In this paper, a size-dependent finite element model, for Mindlin plate theory accounting for the position of the neutral plane for continuum incorporating surface energy effect, is proposed to study the bending behavior of ultra-thin functionally graded (FG) plates. The size-dependent mechanical response is very important while the plate thickness reduces to micro/nano scales. The classical finite element model is adopted to allow insertion of the surface energy into the total energy of the plate. Bulk stresses on the surfaces are required to satisfy the surface balance conditions involving surface stresses. Therefore, unlike the classical continuum plate models, the bulk transverse normal stress is preserved here. Moreover, unlike most of previous studies in the literature, the exact neutral plane position is predetermined and considered for FG plates. A series of continuum governing differential equations which include surface energy and neutral plane position effects are derived. A comparison between the continuum analysis of FG ultra-thin plates with and without incorporating surface energy effects is presented.

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1. Introduction

Atoms at a free surface experience a different local environment than do atoms in the bulk of a material. As a result, the energy associated with these atoms will be different from that of the atoms in the bulk. The excess energy associated with surface atoms is called surface free energy. In classical continuum mechanics, such surface free energy is typically neglected because it is associated with only a few layers of atoms near the surface and the ratio of the volume occupied by the surface atoms and the total volume of material of interest is extremely small. However, for micro/nano-size particles, wires and films, the surface to volume ratio becomes significant, and so does the effect of surface free energy.

Ultra-thin plate structures with submicron thicknesses have attracted much attention due to their potential as sensitive, high frequency devices for applications in Micro-electromechanical Systems (MEMS) and Nano-electromechanical Systems (NEMS) [1–3]. For structures with submicron sizes, due to the increasing surface-to-bulk ratio, surface effects are likely to be significant and can considerably modify macroscopic properties [4,5].

It is known that there exists a size-dependent mechanical response of ultra-thin elastic films with nano-scale thickness [6–9]. The understanding and modeling of such size-dependence due to surface effects is currently of particular interest [10–12].

* Corresponding author. Tel.: +20 122 2232469. E-mail address: ShaatScience@yahoo.com (M. Shaat). Atomistic simulations results have shown that elastic constants of ultra-thin films can be larger or smaller than their bulk counterparts due to the effect of surface energy [13,14]. Furthermore, the elastic constants of the surface may have positive or negative values. In addition, the atomistic lattice model further demonstrates that the values of elastic constants of ultra-thin films are thickness dependent and approach the bulk value as the film thickness increases [15–17]. However, systematic atomistic studies of mechanical response of thin films need tremendous computational efforts; therefore, they are of limited usage in practical applications.

Gurtin and Murdoch [18-21] formulated a generic continuum model of surface elasticity, where the surface of solids can be viewed as a two dimensional elastic membrane with different material constants adhering to the underlying bulk material without slipping. It is found that the continuum by incorporating surface elasticity can predict the same accurate elastic response of thin films similarly as given by the atomistic modeling, if the proper surface constitutive constants are used [8]. Recently, He et al. [10] proposed a rigorous continuum surface elasticity model and successfully analyzed the size-dependent deformation of nano-films. The surface effects on the deflection behavior of ultra-thin films are investigated by incorporating surface elasticity into the Von Karman plate theory without consideration of the non-zero normal stress along the thickness direction [22]. However, the continuum model proposed by Lu et al. [23] takes into account the effect of non-zero normal stress but neglects the effect of nonlinearity. Huang [24] investigated a modified continuum model of elastic films with nano-scale thickness by incorporating surface elasticity into the conventional nonlinear Von Karman Plate theory. A set of governing equations is derived taken into account surface effects, effect of non-zero normal stress and large deflection.

Steigmann and Ogden [25,26] generalized the Gurtin–Murdoch theory to incorporate flexural stiffness of the free surface directly into the constitutive response of surface. Dingreville and Qu [27] investigated the influence of Poisson's ratio effect on the surface properties under general loading conditions. Moreover, the effect of pre-surface tension on the elastic properties of nano structures is studied by Wang et al. [28,29]. In the absence of external loading, the surface pre-tension will induce a residual stress field in the bulk of nano structures. Based on the elastic behavior of nano-sized structural elements such as nano-particles, nano-wires and nano-films, Dingreville [30] investigated an approach for the size dependency of the overall elastic behavior of such nano-sized structural elements.

Functionally graded materials (FGMs) are microscopically inhomogeneous composite materials, in which the volume fraction of the two or more materials is varied smoothly and continuously as a continuous function of the material position along one or more dimension of the structure. The concept of functionally graded material (FGM) was proposed in 1984 by the material scientists in Japan [31]. Alieldin et al. [32] suggested three approaches to transform the laminated composite plate, with stepped material properties, to an equivalent functionally graded (FG) plate with a continuous property function across the plate thickness. Such transformations are used to determine the details of a functionally graded plate equivalent to the original laminated one.

The FGM is suitable for various applications, such as thermal coatings of barrier for ceramic engines, gas turbines, nuclear fusions, optical thin layers, biomaterial electronics, etc. Alibeigloo [33] derived an exact solution for thermo-elastic response of functionally graded rectangular plates subjected to thermomechanical loads. A finite element analysis of thermoelastic field in a rotating FGM circular disk is studied by Afsar and Go [34]. This study focuses on the finite element analysis of thermoelastic field in a thin circular functionally graded material disk subjected to a thermal load and an inertia force due to rotation of the disk. Tung, et al. [35] derived a simple analytical approach to investigate the nonlinear stability of functionally graded plates under mechanical and thermal loads. Equilibrium and compatibility equations for FG plates are derived by using the classical plate theory. Alshorbagy et al. [36] studied the stability of FGMs in high thermal environments. To this aim, a finite element model is presented to study the thermo-elastic behavior of FG plates.

In general, there are many approaches to homogenization of FGM. The choice of the approach should be based on the gradient of gradation relative to the size of a typical representative volume element. Aboudi et al. [37,38] presented studies accounting for local material grading include the constitutive modeling theory based on the higher-order generalized method of cells applied to FGM [37] that was further extended to account for incremental plasticity, creep, and viscoplastic effects in Aboudi et al. [38]. Moreover, a micromechanical analysis of an elastic FGM accounting for the local interaction between the particles and the local gradation effect has recently been conducted by Yin et al. [39]. The subject of the effective thermal conductivity of FGM was also addressed in Yin et al. [40]. The solution includes determining a pairwise thermal interaction followed with a derivation of the averaged heat flux fields of the phases in the particle–matrix zone. The effective thermal conductivity is derived from the relationship between the gradient of temperature and the heat flux distribution.

Mindlin plate theory for continuum incorporating surface energy effects is exploited by Shaat et al. [41] to study the static behavior of ultra-thin FG plates. The transverse shear strain effect is studied by a comparison between the FG plate behavior based on Kirchhoff and Mindlin assumptions. In such analysis the material surface properties are expected to be the same for the upper and lower surfaces of the FG plate. However, the effect of neutral plane position is disregarded for the analysis of the FG plate. A generalized refined theory including surface effects is developed by Lü et al. [42,43] for FG ultra-thin films with different surface properties. The classical generalized shear deformable theory is adopted to incorporate surface energy effects. In such study Lü et al. neglected the effect of neutral plane position on the FG plate behavior.

In this paper, a finite element model is developed to study the behavior of ultra-thin simply supported FG Mindlin plates. Here unlike most of the literatures, [41–43], the effect of the neutral plane position for ultra-thin FG films is investigated. In addition to the effect of the surface energy, the effect of the plate aspect ratio is studied. A set of continuum governing differential equations which include surface energy and neutral plane position effects are derived. A simply supported micro/nano scaled films subjected to a transverse mechanical load are investigated.

2. Mathematical model

In this section, Mindlin plate theory incorporating surface effects is presented. The FG plate is expected to consist of two material constituents. The neutral plane coincides with the geometric mid-plane of isotropic homogenous materials. However, neutral plane of FG plates may not coincide with its geometric mid-plane, because of the material property variation through the plate thickness. In most previous studies, [41–43], the neutral plane is assumed to be coincident with the mid-plane of the plate, while the position of neutral plane for FG plates must be predetermined. To predict the modifications on the classical continuum theory due to taking into account surface energy and neutral plane effects, a series of governing equations are addressed for FG ultra-thin films. Then, the presented governing equations can be solved to study the bending behavior of ultra-thin FG plates.

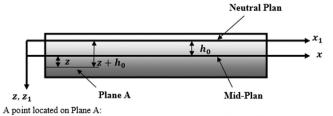
The Mindlin hypothesis is built up on the assumption that the transverse normals do not remain perpendicular to the mid plane after deformation. This amounts to including transverse shear strains in the theory. The inextensibility of transverse normal requires that the vertical deflection ω not be a function of the thickness coordinate z. Under the illustrated assumptions, the displacement field of the first order shear deformation plate theory (FSDT) (Mindlin) is of the form

$$u_{x} = u(x, y, z) = u_{0}(x, y) + (z + h_{0}) \emptyset_{x}(x, y)$$

$$u_{y} = v(x, y, z) = v_{0}(x, y) + (z + h_{0}) \emptyset_{y}(x, y)$$

$$u_{z} = \omega(x, y, z) = \omega_{0}(x, y)$$
(2.1)

where $\{u^0\} = \{u_0, v_0, \omega_0, \varnothing_x, \varnothing_y\}^T$ are unknown functions to be



- 1. Will have (x, z) coordinates with respect to the mid-plane
- 2. Will have $(x, z + h_0)$ coordinates with respect to the neutral plane.

Fig. 1. Coordinate system used for a typical FG plate.

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