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Finite element modeling for elastic nano-indentation problems incorporating surface energy effect

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ABSTRACT

Nano materials have attracted considerable attention during the last two decades, due to their unusual electrical, mechanical and physical properties as compared with their macro counterparts. Mechanical properties of nano materials show strong size-dependency, which has been explained within the framework of continuum mechanics by including the effects of surface residual stresses and surface elasticity as introduced by Gurtin and Murdoch (GM) theory of surface elasticity. In the present work, a finite element model, based on the principle of minimum total potential energy, is developed to monitor the behavior of two-dimensional nano size structures, taking into account the surface effects according to the complete GM model, under elastic frictionless indentation process. Different from most of literature, the presented FE model is capable of solving a variety of problems no matter the complexity of the punch geometry or the boundary conditions. For the sake of comparison as well as validation, the developed model is used for analyzing a simple plane strain problem, and the obtained results have been compared with analytical results published in cited literature. Several problems with different surface-energy model assumptions, indenters of different geometrical shapes and different sizes of indented bodies are solved, to examine its size dependency. The non-conformal contact between the indenter and the elastic half plane is solved, in the context of contact mechanics, by the incremental convex programming (ICP) method.

1. Introduction

Classical elasticity theory was explicitly constructed to be size and time independent. However, recently it was proved that the domain of application of generalized elasticity theory could be considered a formation of some internal characteristic length and time scales of the media for which it is constructed. When these scales are sufficiently small compared to the corresponding external scales then the classical elasticity theories give successful results; otherwise they fail to apply [1]. As an obvious example, for a macro-scale body the surface component of the body is very small relative to the volume of the solid. Thus, we can neglect the surface as a component of the continuum and focus our attention only on the bulk solid. On the contrary, for a nano-scale continuum, the surface is very comparable to the bulk volume. Therefore, its effect should be taken into consider and deserves to be paid a considerable attention to its characteristics and the processes of its interactions with the bulk of the continuum. This may reflect the breakdown of classical continuum mechanics at nano-scale sizes as they were explicitly designed to be size independent. One of the physical reasons for the breakdown of classical continuum mechanics at nano-scale sizes is the surface energy effects. Atomistic simulation results have shown that elastic constants of nano-structural elements can be larger or smaller than their bulk counterparts due to the effect of surface elasticity [2,3]. In addition, the atomistic lattice model further demonstrates that the values of elastic constants of nano-structural elements are size dependent and approach the bulk values as their size increases [4–6]. However, systematic atomistic studies of mechanical response of elastic bodies need tremendous computational efforts; therefore, they are of limited usage in practical applications.

1.1. Surface effect

Gurtin and Murdoch [7–9] formulated a generic continuum model of surface elasticity, where the surface of solids can be viewed as a two dimensional elastic membrane of zero thickness with different material constants adhering to the underlying bulk material without slipping. It is found that the continuum by incorporating residual surface stress and the surface elasticity can predict the same accurate elastic response similarly as given

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by the atomistic modeling, if the proper surface constitutive constants are used. Based on GM surface elasticity model, Miller and Shenoy [10] studied the size-dependent elastic stiffness of some basic structural elements such as nano-bars, nano-beams and nano-plates. Sharma et al. [11,12] studied size-dependent elastic state of three-dimensional nano-inhomogeneities. Yang [13] studied the deformations of an elastic matrix with spherical nano-cavities. Wang and Wang [14] investigated the deformation around a nano-sized elliptical hole with surface effect. Tian and Rajapakse [15,16] obtained the analytical solutions of the size-dependent elastic field of nano-scale circular and elliptical inhomogeneities, respectively. To explore the unconventional mechanical properties of nano-composites and nano-porous materials, Duan et al. [17,18] have taken surface effects and obtained closed-form solutions of elastic state of nano-sized inhomogeneities with spherical and cylindrical shapes. They predicted the effective elastic moduli of nano-composites with uniformly distributed spherical or cylindrical reinforcement using the self-consistency method. Chen et al. [19] also studied elastic solids containing spherical nano-inclusions and derived effective thermal-mechanical properties for such system. Gao and Mahmoud [20] developed a Bernoulli–Euler beam model using the modified couple stress theory and surface elasticity theory.

1.2. Indentation and contact mechanics

The classical problem of an axisymmetric rigid cylindrical or conical punch indenting an elastic half-space first solved by Boussinesq [21]. The problem solution was enhanced for an arbitrary geometry of the punch by Sneddon [22]. From numerical analysis point of view, Conry and Seireg [23] formulated the problem of elastic bodies in frictionless contact as a quadratic programming model. The analysis was restricted to normal surface loading conditions. Bathe and Chaudhary [24] used the Lagrange multiplier method to solve planar, axisymmetric, and 3D frictional contact problems with large deformations. Mahmoud et al. [25] proposed an automated direct method (ADM) for solving the elasto-static frictionless contact problems. The method was based on the solution scheme of nonlinear problem which converts the original nonlinear problem into a series of linear problems by using an incremental technique. Each increment was controlled by activating one of the contact constraint conditions. Mahmoud [26] and Mahmoud et al. [27] extended this procedure to deal with multiphase contact problems. Further, Mahmoud [28] formulated the unbonded frictionless elasto-static contact as a constrained nonlinear programming problem. Furthermore, an incremental procedure to solve the nonconformal unbonded elastic frictionless contact problems was addressed by Mahmoud et al. [29,30]. The problem was formulated as a convex programming model. The model was then updated to accommodate for frictional effect on multiphase contact problem in Mahmoud et al. [31]. However, the model was limited to linear constraints having nonzero coefficients. Therefore, Hassan and Mahmoud [32] extended the model to accommodate these constraints of zero free coefficients.

1.3. Indentation and contact mechanics with surface effect

While analysis of indentation problems have been carried out extensively within the context of classical linear elasticity, based on a careful literature survey, works towards the treatment of surface elasticity to model nano-scale influences in contact problem are still relatively few. However, in the study of elastic contact problems with the surface effect, there are two types of models in most of the existing literature. The first type only considers the residual surface stress while the surface elasticity is neglected (i.e. ignoring surface material constants). For instance, Wang and Feng [33] studied the effect of the residual surface stress on the elastic half-space problem at the nano-scale. Long et al. [34] studied the two-dimensional Hertzian contact problem by considering the effect of the residual surface stress. He and Lim [35] derived the surface Green functions for a soft elastic half-space with surface stress under the assumptions that the soft half-space is impressible and the surface has the same elastic properties as its interior. In their work, only the residual surface stress is considered. On the contrary, the second type only considers the surface elasticity, and the effect of the residual surface pre-stress is neglected. Zhao and Rajapakse [36] obtained analytical solutions for a surface-loaded isotropic elastic layer with surface effects. In their solutions, the residual surface stress does not affect the elastic field in the bulk material. Koguchi [37] formulated three-dimensional surface Green functions for an anisotropic half-domain using the Stroh formalism and considering the anisotropy of the material surface. But, his results have a rather complicated integral form. Chen and Zhang [38] presented the analytical Green's function solutions for an isotropic elastic half-space that was subjected to anti-plane shear deformation. Actually, it can be shown that both the residual surface stress and the surface elasticity are important for the study of the surface effect and that, in general, neither of these effects can be neglected. Nevertheless, in most of the above-mentioned works, only one of these effects was considered. Therefore, nobody can answer the question of whether the contributions of the residual surface stress and of the surface elasticity to the stresses and displacements at the surface are equal or not. In fact, the residual stress is mostly influencing the normal stress, whereas the surface elasticity is dominant factor in the plane shear stress, Wang and Feng [33]. Meanwhile, to simulate accurately the surface effects they adopted the Lagrange description of the governing equations of the surface to express the large strain nature of the surface, Ru [39]. Recently, many authors focused their work on considering the complete GM model in the analysis of nano-scaled indentation problems. For instance, Pinyochotiwong et al. [40] studied analytically, the behavior of nano-structure with complete Gurtin and Murdoch surface model under frictionless indentation process by a rigid punch. Gao et al. [41] demonstrated that residual surface stress and surface elasticity are two equally important parts of surface theory and that, generally, neither of these aspects can be neglected. Finally, Zhou and Gao [42] introduced an analytical solution for the Hertzian and contact problems and other indentation cases with simple indenter geometries and accounting for the surface energy according to the complete GM surface model. It is also noticed that most of these aforementioned papers didn't study the indentation problem in the context of contact mechanics problems. These papers have taken the results of the contact pressure and contact areas from previously published contact mechanics models developed by the classical continuum mechanics, regardless of the surface effects, and exploit it as input data for their indentation models.

1.4. Finite element models for surface effects investigation

For nano-structures with complex geometries and/or complicated constitutive behavior, one has to resort to numerical methods such as the finite element methods to investigate such systems. Gao et al. [43] developed a finite element model to investigate the size-dependent mechanical behavior in nano-systems. Tian and Rajapakse [44] also developed a similar model to study two-dimensional nano-scale inhomogeneities in an elastic matrix. Mahmoud et al. [45] developed a finite element model to study the static bending of nonlocal nano-beams incorporating the surface energy effect. Eltaher et al. [46] extended the work to study the vibrational behavior of nonlocal nano beam