

Effect of Surface Stress on the Deformation around a Nanosized Elliptical Hole: a Finite Element Study

Weifeng Wang, Xianwei Zeng, and Jianping Ding

Abstract—When the characteristic length of an elastic solid is down to the nanometer level, its deformation behavior becomes size dependent. Surface energy /surface stress have recently been applied to explain such dependency. In this paper, the effect of strain-independent surface stress on the deformation of an isotropic elastic solid containing a nanosized elliptical hole is studied by the finite element method. Two loading cases are considered, in the first case, hoop stress along the rim of the elliptical hole induced by pure surface stress is studied, in the second case, hoop stress around the elliptical opening under combined remote tension and surface stress is investigated. It has been shown that positive surface stress induces compressive hoop stress along the hole, and negative surface stress has opposite effect, maximum hoop stress occurs near the major semi-axes of the ellipse. Under combined loading of remote tension and surface stress, stress concentration around the hole can be either intensified or weakened depending on the sign of the surface stress.

Keywords—Surface stress, finite element method, stress concentration, nanosized elliptical hole

I. INTRODUCTION

SIZE-DEPENDENT deformations of nanosized materials and structures have attracted considerable experimental and theoretical studies in recent years. Different from bulk materials, the effects of surfaces on mechanical deformations of nano-structured materials become important as the ratio of the number of surface atoms to total atoms increases sharply. To address the size-dependent mechanical behavior of nanosized materials and structures, the contribution of the surface free energy to the total free energy of a nano-system need to be considered. In the 1970s, Gurtin and Murdoch [1, 2] proposed a surface stress model to account for the effect of surface energy on elastic deformation within the framework of classical continuum mechanics. Recently the Gurtin and Murdoch surface stress model has been applied to study various elasticity

problems involving nano-sized materials and structures. This usually leads to nonconventional boundary value problem in Elasticity.

To this end, Miller and Shenoy [3] studied the size-dependent elastic stiffness of structural elements such as nanobars, nanobeams and nanoplates; Sharma et al. [4,5] studied size-dependent elastic state of three-dimensional spherical and ellipsoidal nano-inhomogeneities; Yang [6] investigated the deformation of an elastic matrix with spherical nanocavities; Wang and Wang [7] obtained the closed-form solution of the deformation around a nanosized elliptical hole with surface effect using the complex variable formulation and the conformal mapping technique; Tian and Rajapakse [8,9] obtained the analytical solutions of the size-dependent elastic field of a nanoscale circular and an elliptical inhomogeneities respectively using the complex variable formulation and the Laurent series. Ou et al. [10] investigate the effect of residual surface tension on the stress concentration around a nanosized spheroidal cavity using the method of Boussinesq-Sadowsky's potential functions. Moreover, Duan et al. [11,12] obtained closed-form solutions of elastic state of nanosized inhomogeneities with spherical and cylindrical shapes, and predicted the effective elastic moduli of nanocomposites with uniformly distributed spherical or cylindrical reinforcement using the self-consistency method; Chen et al. [13] also studied elastic solids containing spherical nano-inclusions and derived effective thermal-mechanical properties for such system.

Note that the above mentioned studies are restricted to nanosystems with simple geometries, i.e. an infinite isotropic elastic medium with inhomogeneities of ideal shape such as cylindrical or spherical. Even for problems involving such simple geometries, analytical solutions to such problems are nontrivial and they are of very complicated forms. These complicated analytical solutions need to be verified by numerical studies and/or experimental studies. Simple closed form solutions are possible for inhomogeneities with constant curvature such as spheres and circular cylinders. However, for inhomogeneities with non-uniform curvature such as elliptical cylinders, simple closed form solutions are rare. Though Wang and Wang [7] claimed that they had obtained a closed-form solution for the deformation around a nanosized elliptical hole with surface tension, their analytical is not correct as it will be shown in ensuing sections of this paper. The Gurtin and

Weifeng Wang is a professor with the School of Civil Engineering and Transportation, South China University of Technology, Guangzhou, 510640, China (e-mail: ctwfwang@scut.edu.cn).

Xianwei Zeng is an associate professor with the School of Civil Engineering and Transportation, South China University of Technology, Guangzhou, 510640, China (phone: +86.20.87110804; fax: +86.20.87114460; e-mail: zengxw@scut.edu.cn).

Jianping Ding is with the College of Materials Science and Engineering, South China University of Technology, Guangzhou, 510640, China (e-mail: jpding@scut.edu.cn).

Murdoch surface stress model has also been incorporated into finite element programs for the investigation of size-dependent deformations of nanosystems. For example, Gao et al. [14] developed an in-house finite element code to investigate the size-dependent mechanical behavior of nanosystems and Tian and Rajapakse [15] developed a similar program to study two-dimensional nanoscale inhomogeneities in an elastic matrix. Those in-house codes lack the handy pre- and post-processing capabilities and material and geometrical nonlinearities as those included in general finite element codes such as ANSYS, ABAQUS, etc.

The objective of this study is to investigate the effect of surface tension on the plane strain deformation around an elliptical hole in an isotropic elastic solid by the finite element method. The general finite element code ABAQUS is used in the analysis. Two loading cases are considered, in the first case, the elastic deformation due to surface tension only on the rim of the elliptical hole is considered; whereas in the second case, the elastic deformation due to combined remote tension and surface tension on the rim of the hole is considered. Numerical results for the hoop stress along the rim of the elliptical hole is compared available analytical results in the literature [7].

II. AN ISOTROPIC ELASTIC SOLID WITH AN ELLIPTICAL HOLE

Consider the plane strain deformation of an infinite isotropic elastic solid containing a nanosized elliptical hole as shown in Fig. 1. The major and minor semi-axes of the ellipse are a and b respectively. The solid is subjected to remote tension σ_0 parallel to the y -axis and uniform surface tension γ on the rim of the elliptical hole. In the absence of body force, the equilibrium equation at a material point inside the bulk is given by,

$$\sigma_{ij,j} = 0 \quad (i, j = 1, 2) \quad (1)$$

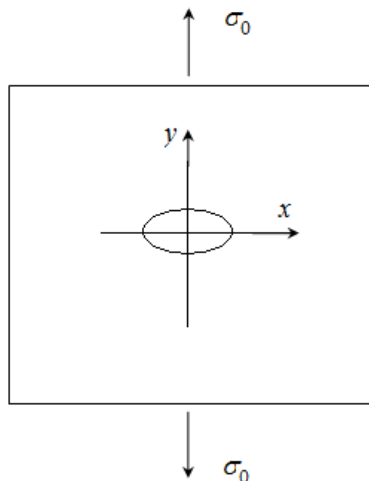


Fig. 1 A nanoscale elliptical hole in an isotropic elastic solid.

where σ_{ij} is the stress tensor. Assuming the surface is negligibly thin and adhering to its neighboring bulk material without slipping, the equilibrium equation of a material point on the surface of the hole is given by [1, 2],

$$\begin{aligned} \sigma_{\alpha\beta,\beta}^s + \sigma_{\alpha\beta} n_\beta &= 0 \\ \sigma_{\alpha\beta}^s k_{\alpha\beta} &= \sigma_{ij} n_i n_j \quad (i, j = 1, 2, \alpha, \beta = 1, 2) \end{aligned} \quad (2)$$

where $\sigma_{\alpha\beta}^s$ is the surface stress, $k_{\alpha\beta}$ the curvature of the surface, and n_i the unit normal to the surface.

Assuming isotropic and linear elastic, the constitutive relations for a material point inside the bulk is,

$$\sigma_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} \quad (i, j = 1, 2) \quad (3)$$

where ε_{ij} is the strain tensor, λ and μ are the Lamé's constants and δ_{ij} denotes the Kronecker delta.

The surface stress tensor $\sigma_{\alpha\beta}^s$ is related to the surface energy density γ by the Shuttleworth's equation [16],

$$\sigma_{\alpha\beta}^s = \gamma \delta_{\alpha\beta} + \frac{\partial \gamma}{\partial \varepsilon_{\alpha\beta}} \quad (4)$$

where $\varepsilon_{\alpha\beta}$ is the surface strain tensor. In this study, only the case such that the surface energy density is independent of surface strain is considered.

For a nanoscale system under infinitesimal deformation, the strain tensor ε_{ij} ($i, j = 1, 2$) is related to the displacement vector u_i ($i = 1, 2$) by the following kinematic equation,

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (5)$$

The traction boundary condition for the nanosystem shown in Fig.1 is ,

$$\sigma_{yy} = \sigma_0 \quad \text{at remote} \quad (6)$$

III. FINITE ELEMENT MODELING AND NUMERICAL RESULTS

In view of eqns. (2) and (4), for the case such that the surface energy density is independent of surface strain, the boundary value problem shown in Fig. 1 is equivalent to the problem of an elliptical hole inside an infinite isotropic elastic solid subjected to remote traction σ_0 , zero shear traction on the surface of the elliptical hole and a non-uniform normal traction related to the curvature of the elliptical hole such that,

$$\begin{aligned} \sigma_{\xi\eta} &= 0 \\ \sigma_{\xi\xi} &= \frac{\gamma}{\rho} \end{aligned} \quad (7)$$

where ρ is the curvature radius of the elliptical hole which can be expressed as,

$$\rho = R \frac{(1 + m^2 - 2m \cos(2\theta))^{3/2}}{1 - m^2} \quad (8)$$

where $R=(a+b)/2$, $m=(a-b)/(a+b)$, and θ is determined such that the contour of the ellipse can be described by the coordinates $x=acos(\theta)$ and $y=bsin(\theta)$.

In this study, the general finite element code ABAQUS is used to model the elasticity problem shown in Fig. 1, the infinite plane is approximated by a square of its width equals to 20 times that of the major semi-axis a . Due to symmetry, only a quarter of the solid is modeled (Fig. 2). Finite element mesh is refined near the major semi-axis. The non-uniform normal traction [eqn. (7)] on the boundary of the elliptical hole can be imposed through the user subroutine DLOAD in ABAQUS.

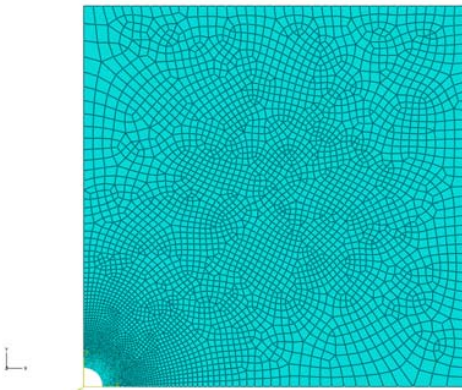


Fig. 2 (a) Finite element mesh corresponding to $m=0$.

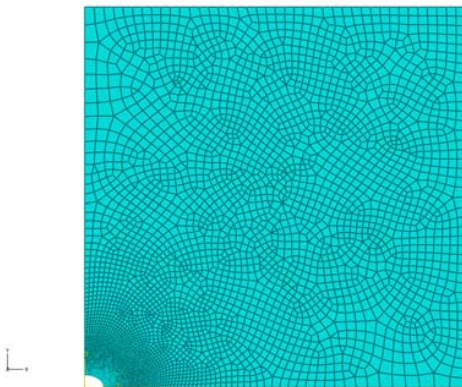


Fig. 2 (b) Finite element mesh corresponding to $m=0.2$.

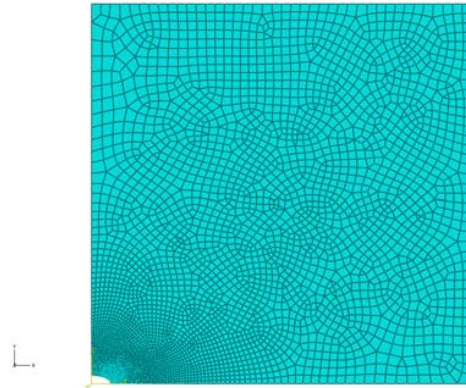


Fig. 2 (c) Finite element mesh corresponding to $m=0.4$.

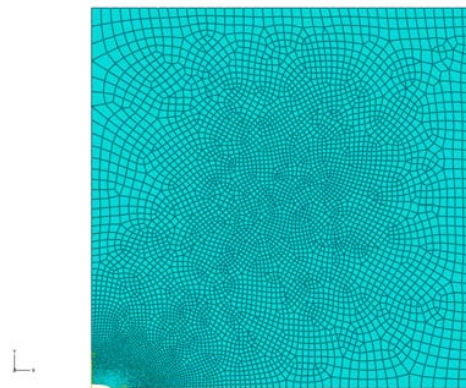


Fig. 2 (d) Finite element mesh corresponding to $m=0.6$.

3.1 Surface stress Induced Hoop Stress

To highlight the effect of surface stress on the deformation around a nanosized elliptical hole, hoop stress along the elliptical hole induced by strain independent surface stress γ only is shown in Fig. 3 (a), for elliptical holes with different shapes ($m=0, 0.2, 0.4$ and 0.6). For comparison, analytical solutions obtained by Wang and Wang [7] are shown in Fig. 3(b). They showed that the summation of the hoop stress and the normal stress along the elliptical hole is zero, and hence the hoop stress is given by,

$$\sigma_{\eta\eta} = -\left(\frac{\gamma}{R}\right) \frac{1 - m^2}{(1 + m^2 - 2m \cos(2\theta))^{3/2}} \quad (9)$$

It is revealed by the finite element results shown in Fig. 3(a) that the simple closed form solution of the hoop stress obtained by Wang and Wang [7] (eqn. (9)) is incorrect; solution to this elasticity problems does not admit such a simple form. According to the finite element analysis, positive surface stress induces negative hoop stress, while negative surface stress induces positive hoop stress. Maximum hoop stress

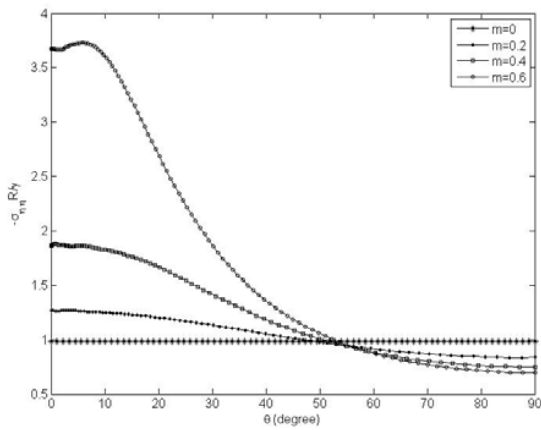


Fig. 3 (a) Distribution of the hoop stress along the elliptical hole induced by surface stress (FEM results by ABAQUS).

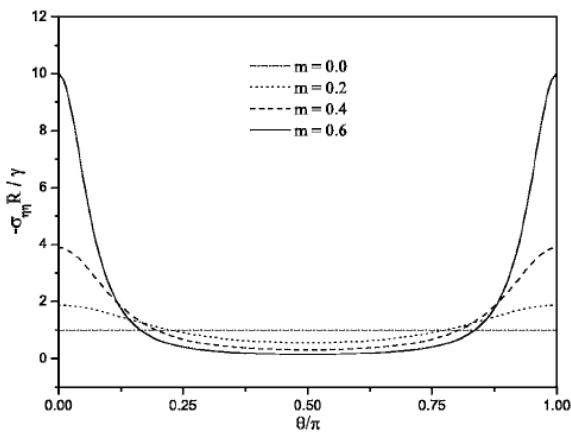


Fig. 3 (b) Distribution of the hoop stress along the elliptical hole induced by surface stress (analytical results by Wang and Wang [7]).

occurs near the major semi-axis of the elliptical hole, but not necessary on the major semi-axis where the curvature is maximum. The magnitude of the hoop stress is highly affected by the geometry of the elliptical hole (R and m). When $m=0$, the ellipse is reduced to a circle, the hoop stress is constant. According to Wang and Wang’s analytical results, maximum hoop stress always occurs at the major semi-axis of the elliptical hole where the curvature is maximum. This is not true as shown by the present finite element results.

3.2 Effect of Surface stress on the hoop stress around the elliptical hole when subjected to remote loading

To study the effect of surface stress on the stress concentration near an elliptical hole, the hoop stress along an elliptical hole induced by remote loading combined with strain independent surface stress γ of different magnitudes is studied. Numerical results shown in the sequel corresponds to an elliptical hole with $m=0.5$. Fig. 4 shows the finite element mesh of a quarter of the structure. FE results for the hoop stress is

shown in Fig. 5 (a), and the analytical solutions obtained by Wang and Wang [7] are shown in Fig. 5(b) respectively. They showed that the hoop stress is given by the following equation,

$$\sigma_{\theta\theta} = -\left(\frac{\gamma}{R}\right) \frac{1 - m^2}{(1 + m^2 - 2m \cos(2\theta))^{3/2}} + \sigma^0 \frac{1 - m^2 + 2 \cos(2\theta) - 2m}{1 + m^2 - 2m \cos(2\theta)} \quad (10)$$

As shown in Fig. 5(a) and Fig. 5(b), the simple closed form solution of the hoop stress obtained by Wang and Wang [7] (eqn. (10)) is incorrect; solution to this elasticity problem does not admit such a simple form. The stress concentration around the elliptical hole can be either intensified or weakened depending on the sign of the surface stress. Positive surface stress weakens the stress concentration along the hole, while negative surface stress increases the stress concentration around the hole. For the surface stress level considered in Fig. 5, the maximum hoop stress always occurs at the major semi-axis of the ellipse.

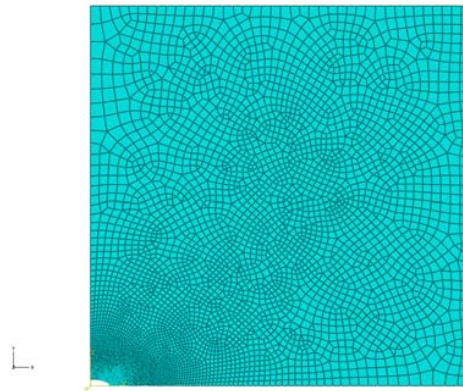


Fig. 4 Finite element mesh corresponding to $m=0.5$.

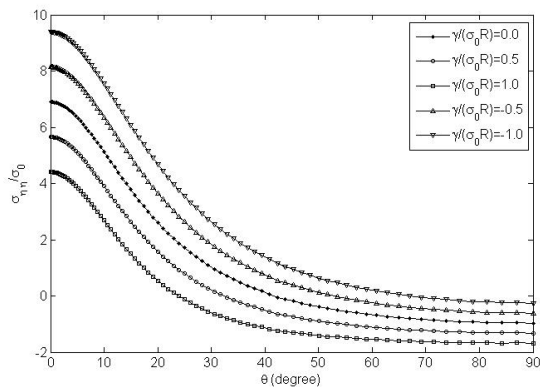


Fig. 5 (a) Effect of surface stress on the hoop stress along the elliptical hole subjected to remote loading (FEM results by ABAQUS).

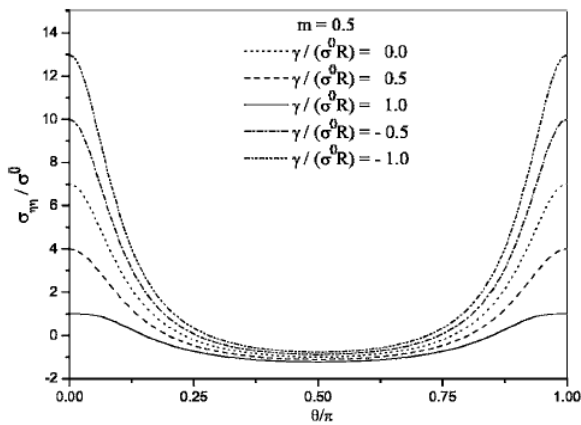


Fig. 5 (b) Effect of surface stress on the hoop stress along the elliptical hole subjected to remote loading (analytical results by Wang and Wang [7]).

IV. CONCLUSIONS

The effect of strain-independent surface stress on the deformation of an isotropic elastic solid containing a nanosized elliptical hole is studied by the finite element method. Two loading cases are considered, in the first case, hoop stress along the elliptical hole induced by surface stress only is investigated. It has been shown that positive surface stress induces negative hoop stress, and vice versa. Maximum hoop stress occurs near the major semi-axis of the elliptical hole, but not necessary at the major semi-axis where the curvature is maximum. The magnitude of the hoop stress is affected by the geometry of the elliptical hole (R and m). In the second case, hoop stress around the elliptical hole under combined remote loading and surface stress is investigated. The stress concentration around an elliptical hole can be either intensified or weakened depending on the sign of the surface stress. Positive surface weakens the stress concentration along the hole, while negative surface stress increases the stress concentration. For sufficiently small surface stress, the maximum hoop stress always occurs at the major semi-axis of the ellipse. Numerical results presented in this paper show that the simple closed form solution available in the literature [7] is incorrect. This simple elasticity problem involving surface stress does not admit such a simple analytical solution.

ACKNOWLEDGMENT

This work was supported by a start-up grant from South China University of Technology under the second phase of '985 Project'.

REFERENCES

- [1] M. E. Gurtin, and A. I. Murdoch, "A continuum theory of elastic material surfaces," *Arch. Ration. Mech. Anal.*, vol. 57, pp. 291-323, 1975.
- [2] M. E. Gurtin, and A. I. Murdoch, "Surface stress in solids," *Int. J. Solids and Struct.*, vol.14, pp. 431-440, 1978.
- [3] R. E. Miller, and V. Shenoy, "Size-dependent elastic properties of nanosized structural elements," *Nanotechnology*, vol. 11, pp. 139-147, 2002.
- [4] P. Sharma, S. Ganti, and N. Bhate, "Effect of surfaces on the size-dependent elastic state of nano-inhomogeneities," *Applied Physics Letters*, vol. 82, pp.535-537, 2003.
- [5] P. Sharma P, and S. Ganti, "Size-dependent Eshelby's tensor for embedded nano-inclusions incorporating surface/interface energies," *J. Applied Mechanics*, vol. 71, pp. 663-671, 2004.
- [6] F. Yang, "Size-dependent effective modulus of elastic composite materials: spherical nanocavities at dilute concentrations," *J. Applied Physics*, vol. 95, pp. 3516-3520, 2004.
- [7] G. F. Wang, and T. J. Wang, "Deformation around a nanosized elliptical hole with surface effect," *Applied Physics Letters*, vol. 89: pp. 161901-161903, 2006.
- [8] L. Tian L, and R. K. N. D. Rajapakse, "Analytical solution for size-dependent elastic field of a nanoscale circular inhomogeneity," *J. Applied Mechanics*, vol. 74, pp. 568-574, 2007.
- [9] L. Tian L, and R. K. N. D. Rajapakse, "Elastic field of an isotropic matrix with a nanoscale elliptical inhomogeneity," *Int. J. Solids Struct.*, vol. 44, pp. 7988-8005, 2007.
- [10] Z. Y. Ou, G. F. Wang, and T. J. Wang, "Effect of residual surface tension on the stress concentration around a nanosized spheroidal cavity," *Int. J. Engrg. Sci.*, vol. 46, pp. 475-485, 2008.
- [11] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karihaloo, "Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress," *J. Mech. Phys. Solids*, vol. 53, pp. 1574-1596, 2005.
- [12] H. L. Duan, J. Wang, B. L. Karihaloo, and Z. P. Huang, "Nanoporous materials can be made stiffer than non-porous counterparts by surface modification," *Acta Mater.*, vol. 54, pp. 2983-2990, 2006.
- [13] T. Chen, G. J. Dvorak, and C. C. Yu, "Solids containing spherical nano-inclusions with interface stresses: effective properties and thermal-mechanical connections," *Int. J. Solids Struct.*, vol. 44, pp. 941-955, 2007.
- [14] W. Gao, S. W. Yu, and G. Y. Huang, "Finite element characterization of the size-dependent mechanical behavior in nanosystems," *Nanotechnology*, vol. 17, pp. 1118-1122, 2006.
- [15] L. Tian, and R. K. N. D. Rajapakse, "Finite element modeling of nanoscale inhomogeneities in an elastic matrix," *Computational Materials Science*, vol. 41, pp. 44-53, 2007.
- [16] R. C. Cammarata, "Surface and interface stress effects in thin film," *Prog. Surf. Sci.*, vol. 46, pp. 1-38, 1994.