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Finite Element Modeling of two-dimensional Nanoscale Structures with Surface Effects

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***Abstract*—**Nanomaterials have attracted considerable attention during the last two decades, due to their unusual electrical, mechanical and other physical properties as compared with their bulky counterparts. The mechanical properties of nanostructured materials show strong size dependency, which has been explained within the framework of continuum mechanics by including the effects of surface stress. The size-dependent deformations of two-dimensional nanosized structures with surface effects are investigated in the paper by the finite element method. Truss element is used to evaluate the contribution of surface stress to the total potential energy and the Gurtin and Murdoch surface stress model is implemented with ANSYS through its user programmable features. The proposed approach is used to investigate size-dependent stress concentration around a nanosized circular hole and the size-dependent effective moduli of nanoporous materials. Numerical results are compared with available analytical results to validate the proposed modeling approach.

***Keywords*—**Nanomaterials, finite element method, size dependency, surface stress

I. Introduction

NANOSTRUCTURED materials have been shown to possess unusual electrical, mechanical and other physical properties as compared with their bulky counterparts. For example, Jing et al. [1] recently measured the Young's modulus of silver nanowires by three-point bending test using contact force microscopy. The Young's modulus was shown to have strong size dependency, .i.e. the modulus for a nanowire with a diameter of 20 nm doubles that with a diameter of 140 nm. The size dependency has been attributed to the effects of surface elasticity and residual surface stress. In nanostructured materials, the effects of surface/interface on their mechanical deformation become important as the area of surface/interface to bulk volume increases sharply when compared with conventional materials. Moreover, since the atoms on the surface/interface have different equilibrium configuration from the atoms in the bulk, the elastic stiffness of the surface can be different from those of the bulk. To address the size-dependent mechanical behaviour of nanosized structures, the contribution of the surface/interface free energy to the total free energy of a nanosized structure need to be considered. To this end, classical continuum mechanics needs to be modified to account for the effects of surface/interface on deformation. Gurtin and Murdoch [2, 3] proposed a linear surface stress model, where the surface stress is a linear function of the surface strain and the surface is assumed to have null thickness with different elastic modulus from the bulk. The Gurtin and Murdoch surface stress model has recently been extensively applied to investigate a variety of mechanics problems involving nanomaterials and nanostructures.

Based on the Gurtin and Murdoch surface stress model, Miller and Shenoy [4] studied the size-dependent elastic stiffness of some basic structural elements such as nanobars, nanobeams and nanoplates; Sharma et al. [5,6] studied size-dependent elastic state of three-dimensional nano-imhomogeneities; Yang [7] studied the deformations of an elastic matrix with spherical nanocavities; Wang and Wang [8] investigated the deformation around a nanosized elliptical hole with surface effect; Tian and Rajapakse [9,10] obtained the analytical solutions of the size-dependent elastic field of a nanoscale circular and an elliptical imhomogeneities respectively. To explore the unconventional mechanical properties of nanocomposites and nanoporous materials, Duan et al. [11,12] obtained closed-form solutions of elastic state of nanosized imhomogeneities 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.

The above mentioned studies are restricted to nanosystems with simple geometries, i.e. an infinite isotropic elastic medium with imhomogeneities of ideal shape such as cylindrical or spherical. For nanostructures with complex geometries, and/or more complicated constitutive behaviour, one has to resort to numerical methods such as the finite element methods to investigate such systems. To this end, Gao et al. [14] developed an in-house finite element code to investigate the size-dependent mechanical behaviour in nanosytems; Tian and Rajapakse [15] also developed a similar program to study two-dimensional nanoscale imhomogeneities 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

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such as ANSYS, ABAQUS, etc., it is ideal to devise an alternative approach to model nanoscale materials with surface stress effects. This is the objective of the present study. The governing equations for a two-dimensional nanoscale structure are presented in Section 2; followed by finite element formulation and implementation with the finite element code ANSYS in Section 3 and numerical results on size-dependent elastic state of nanoholes and effective moduli of nanoporous materials are presented in Section 4.

II. Governing Equations And Boundary Conditions

Consider the plane strain deformation of a two-dimensional solid containing nanosized holes and imhomogeneities as shown in Fig. 1. Both the matrix and the imhomogeneities are assumed to be isotropic and linear elastic. For more complicated cases involving material and geometrical nonlinearities, the equations shown in the sequel sections need to be modified accordingly. The equilibrium equation at a material point inside the matrix or the imhomogeneity can be expressed as,

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

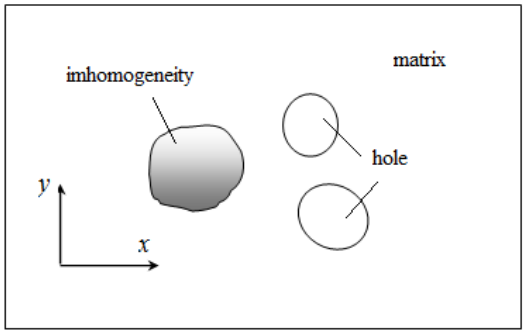

Fig. 1 Two dimensional plane with nanoscale holes and imhomogeneities

where σ_{ij} and b_i denote stress and body force, respectively. Assuming the surface or the interface is negligibly thin and adhering to its neighbouring bulk material without slipping, the equilibrium equation of a material point on a surface/interface is given by [2,3],

$$\begin{aligned} &\sigma^s_{\alpha\beta,\beta} + \left[\sigma_{\alpha\beta} n_\beta\right] = 0 \\ &\sigma^s_{\alpha\beta} k_{\alpha\beta} = \left[\sigma_{ij} n_i n_j\right] \quad (i, j = 1,2, \alpha, \beta = 1,2) \end{aligned} \tag{2}$$

where $\sigma^s_{\alpha\beta}$ denotes the surface/interface stress, $k_{\alpha\beta}$ the curvature of the surface/interface, n_i the normal to the surface/interface and the bracket '[ ]' refers to the jump of quantities across the surface/interface.

Assuming isotropic and linear elastic, the constitutive behaviour for a material point inside the matrix or imhomogeneity is,

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

where ε_{ij} is the strain tensor, λ and μ are the Lame's constants and δ_{ij} denotes the Kronecker delta.With regard to the material behaviour for a surface/ interface, Gurtin and Murdoch proposed a linear surface stress-surface strain model for a general three-dimensional surface/interface [10],

$$\sigma^s_{\alpha\beta} = \tau^0 \delta_{\alpha\beta} + 2\left(\mu^s - \tau^0\right)\varepsilon_{\alpha\beta} + \left(\lambda^s + \tau^0\right)\varepsilon_{kk}\delta_{\alpha\beta} \quad (\alpha, \beta = 1,2) \tag{4}$$

where $\varepsilon_{\alpha\beta}$ denotes the surface strain, λ^s and μ^s are the Lame's constants of a surface or an interface and τ^0 is the residual surface/interface stress at zero strain.For the two-dimensional problem considered in the present study, the Gurtin and Murdoch surface/interface stress model is further reduced to,

$$\sigma^s = E^S \varepsilon^S + \tau^0 \tag{5}$$

where σ^s and ε^s denote the surface stress and surface strain in two-dimensional case, respectively, and $E^s\,(=\lambda^s + 2\mu^s - \tau^0)$ is the reduced elastic modulus for 2D case.

For a nanoscale system under infinitesimal deformation, the strain tensor $\varepsilon_{\alpha\beta}$ is related to the displacement u_α $(\alpha = 1,2)$ by the following kinematic equation,

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{6}$$

The boundary conditions for the nanosystem shown in Fig.1 include displacement and/or traction boundary conditions such as,

$$\begin{aligned} &u_i = \bar{u}_i \quad \text{on } \Gamma_u \\ &\sigma_{ij} n_j = t_i \quad \text{on } \Gamma_t \end{aligned} \tag{7}$$

where Γ_u and Γ_t denote boundaries with specified displacement and traction boundary conditions, respectively.

III. Finite Element Formulation And Implementation

A complete boundary value problem (BVP) governing the deformation of a two-dimensional nanosized structure with holes and imhomogeneities is defined in the previous section. The analytical solution to the above boundary value problem is a nontrivial task, except for an infinite plane with circular or elliptical holes or imhomogeneities. In this section, a displacement-based finite element approach is proposed to numerically solve the BVP with surface stress. To this end, the BVP described by partial differential equations is transformed into an equivalent energy statement, i.e. by assuming admissible displacement field satisfying the kinematic (6) and the displacement boundary conditions in (7), the actual displacement field to the BVP should minimize the total potential energy of the nanosystem. The total potential energy of the system (Π) can be obtained by the summation of the strain energy of the bulk material (U^b), the strain energy of the surface/interface (U^s) and the work by external force (W) as,

$$\Pi = U^b + U^s + W \tag{8}$$

The potential energy of the bulk material is given by,

$$U^b = \iint_V \frac{1}{2}\{\varepsilon\}^T [D]\{\varepsilon\} dV \tag{9}$$

where $\{\varepsilon\}$ is the strain vector and [D] is the elasticity matrix of the bulk material, which is different for the matrix and the inhomogeneity. The potential energy of a surface/interface with linear surface stress-strain relationship (5) is given by,

$$U^s = \int_S \frac{1}{2} E^s (\varepsilon^s)^2 dS + \int_S \tau^0 \varepsilon^s dS \tag{10}$$

Since the surface/interface is assumed to be adhering to the bulk material without slipping or opening, the surface strain can be related to the strain vector of the bulk material through a coordinate transformation matrix [T],

$$\varepsilon^s = [T]\{\varepsilon\} \tag{11}$$

The work done by external body force {b} and surface tractions {t} is given by,

$$W = -\iint_V \{u\}^T \{b\} dV - \int_{\Gamma_t} \{u\}^T \{t\} d\Gamma \tag{12}$$

where $\{u\}$ denotes the displacement vector.

In displacement-based finite element analysis, the displacement field within an element is approximated by piece-wise interpolation such as,

$$\{u\} = [N]\{a\} \tag{13}$$

where [N] is the shape function matrix and {a} is the nodal displacement vector. The strain vector of the bulk material is related to the nodal displacement vector as,

$$\{\varepsilon\} = [B]\{a\} \tag{14}$$

where [B] is the strain-displacement matrix.

By substituting the displacement vector, strain vector and the surface strain into the total potential energy (Π) and invoking the stationary condition ($\delta\Pi = 0$), the finite element equilibrium equation is finally derived as,

$$[K]\{a\} = \{f\} \tag{15}$$

where the total stiffness matrix [K] is,

$$[K] = \iint_V [B]^T [D][B] dV + \int_S [B]^T [T] E^s [T][B] dS \tag{16}$$

and the force vector {f} can be expressed as,

$$\{f\} = \iint_V [B]^T \{b\} dV + \int_{\Gamma_t} [B]^T \{t\} d\Gamma + \int_S [B]^T [T]^T \tau^0 dS \tag{17}$$

It is clearly identified from (16) and (17) such that, due to the presence of surface/interface stress, both the stiffness matrix and the force vector will change. The elastic stiffness of a surface/interface has a contribution on the total stiffness matrix while the residual stress/interface stress has an effect on the force vector. For a nanosized structure, the effects of surface/interface stress on its elastic state can be remarkable when compared with those on macroscopic structure. In conventional finite element analysis of a macroscopic structure, the contribution of surface/interface on deformation is negligible.

In order to calculate the contributions of surface/interface stress to the total stiffness matrix and the force vector, Gao et al. [14] developed an in-house finite element code with four-node quadrilateral element for the bulk and two-node element for the surface and Tian and Rajapakse [15] developed an in-house code with eight-node isoparametric bulk elements and three-node element for the surface. Note that those in-house codes lack powerful pre- and post-processors and capabilities to handle material and geometrical nonlinearities, it is more desirable to investigate the contributions of surface/interface stress with general-purpose finite element codes such as ANSYS, ABAQUS etc. In this study, a novel approach is proposed here to handle surface/interface stress within the scope of ANSYS. If the matrix and the imhomogeneity are partitioned with 4-node quadrilateral elements, the surface/interface is essentially discreetized into two-node segements. In such a case, the contribution of each two-node surface/interface segment to the total stiffness matrix can be evaluated by integrating the second term of (16) and its explicit form in the local coordinate system pointing from one node to the other is determined as,

$$[K^S]^e = \frac{E^S}{L^e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{18}$$

where $[K^s]^e$ denotes the element stiffness matrix of a two-node surface/interface segment, and L^e is the distance between the two-node. Note that in finite element analysis, the element stiffness matrix of a two-node truss element is,

$$[K]^e = \frac{EA}{L^e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{19}$$

where E and A denotes the Young's modulus and the cross sectional area of the truss element, respectively.

Therefore, the contribution of the surface/interface to the total stiffness matrix of a nanosystem can be modeled by fictitious truss element provided that $E^S = EA$ is satisfied. Note that in conventional finite element program, the young's modulus of a truss cannot be negative. However, recently studies have shown that the elastic modulus of a surface can be positive or negative depending on the surface crystal orientation [4]. Therefore, surface having negative modulus cannot be simulated using the truss element in conventional finite element codes. Fortunately, ANSYS's user programmable features (UPFs) allow one to compile and link user subroutines to the ANSYS program [16], resulting in a user version finite element program. The details of ANSYS user programmable features can be found in Ref. [16]. In order to model the linear surface/interface stress model (5), an user subroutine called 'usermat.f' has been developed in the course of the study. Since the conventional truss element 'LINK1' in ANSYS is not allowed to invoke the user subroutine 'usermat.f', the truss element 'LINK180' is employed to model the surface/interface. In such a manner, one can model an elastic surface/interface with either positive or negative modulus.

IV. Numerical Results

In this section, stress concentration around a nanosclae circular hole under remote loading and the effective moduli of two-dimensional solid containing circular nanovoids are investigated to highlight the effects of surface stress. Numerical results are obtained using the finite element program ANSYS combined with the developed user subroutine 'usermat.f'. To model the effects of surface stress, the elastic moduli of a surface are prerequisite. To this end, Miller and Shenoy [4] calculated the surface elastic constants of Aluminum using the embedded atom method (EAM) and reported that the surface elastic constants depend on the material type and the surface crystal orientation. For Al [100] surface, λ^s =3.4939 N/m, μ^s = -5.4251 N/m and τ^0 =0.5689 N/m and For Al [111] surface, λ^s =6.8511 N/m, μ^s = -0.3760 N/m and τ^0 =0.9108 N/m. These surface elastic constants are used in the ensuing sections, unless otherwise specified.

A. Stress Concentration Around A Circular Hole

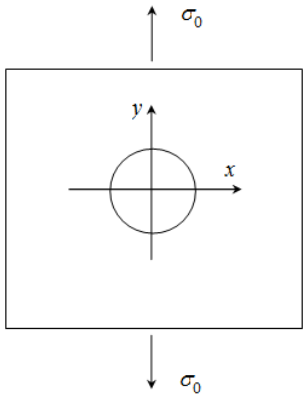

Fig. 2 A nanoscale circular hole in an infinite plane

Consider the plane strain deformation of an infinite material plane containing a nanosized circular hole of radius a under uniaxial remote traction σ^0 as shown in Fig. 2. The material considered here is Aluminum with elastic constants: λ =58.17 GPa and μ =26.13 GPa. Due to the presence of the circular hole, stress concentration occurs around the hole. The analytical solution to this problem was given by Tian and Rajapakse [9] and the stress concentration factor was obtained as,

$$S_c = 3 - \frac{(\Lambda_1\Lambda_2 + 2\Lambda_1)}{2(1+2\Lambda_1)} - \frac{3(\Lambda_1\Lambda_2 + 2\Lambda_1)}{1+4\Lambda_1+\Lambda_1\Lambda_2} \quad (20)$$

where $\Lambda_1 = E^s / 4\mu a$ and $\Lambda_2 = 2\mu/(\lambda+\mu)$ .The above analytical solution is used to validate the proposed modeling approach with ANSYS. Fig. 3 shows the variation of the stress concentration factor with the hole radius for both positive and negative surface Young's modulus E^s (residual surface stress τ^0 is assumed to be zero).

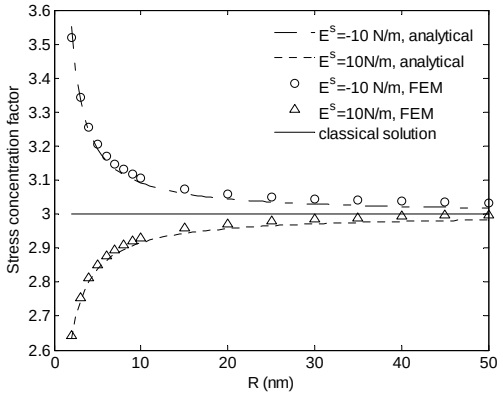

Fig. 3 Variation of the stress concentration factor with the hole radius R

As shown in Fig.3, the classical stress intensity factor is independent of the hole size, while the stress concentration factor for a nanoscale hole is highly size-dependent. For a circular hole with positive surface elastic modulus, the stress concentration is reduced compared with classical elasticity solution and it is increasing with increasing hole size. On the contrary, for a hole with negative surface modulus, the stress concentration is increased when compared with classical solution and it is decreasing with increasing hole size. For surface with either positive or negative elastic modulus, the stress concentration factor tends to the classical solution when the hole radius is greater than 20nm. The present numerical results well agree with the analytical solutions and this confirms the validity of the proposed approach for modeling nanoscale structures with surface effects.

B. Effective Moduli of Nanoporous Material with Circular Voids

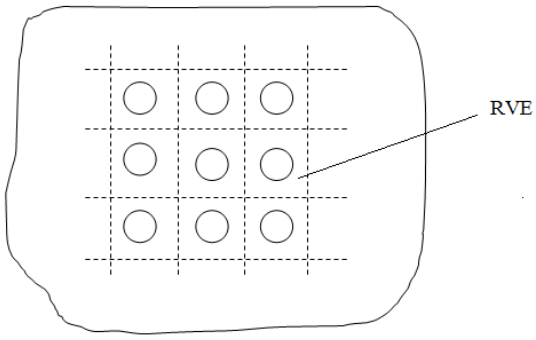

Fig. 4 Nanoporous materials with square representative volume element (RVE)

Recently there is much interest in the development and understanding of nanocomposites and nanoporous materials. To design macroscopic structures with nanocomposites and nanoporous materials, their effective elastic moduli are important parameters. To this end, the effective moduli of a

nanocomposite can be predicted by various homogenizing procedure such as the self-consistent method, using the properties of the matrix, the reinforcement and the interface. Similarly, the effective moduli of a nanoporous material can be predicted with the properties of the matrix and the surface. Consider the case of a two dimensional material plane with periodically distributed nanoscale circular voids shown in Fig. 4. The material for the matrix is Aluminum with elastic constants: λ =58.17 GPa and μ =26.13 GPa and surfaces with different elastic constants are considered: for Type A surface, λ^s =3.4939 N/m, μ^s = -5.4251 N/m and for Type B surface, λ^s =6.8511 N/m, μ^s = -0.3760 N/m. For both surface types, the residual surface stress is assumed to be zero.

To predict the effective properties of the nanoporous material using the finite element method, a representative volume element (RVE) is identified first. The effective moduli provide a link between the average stress and the average strain in the RVE. One commonly used approach to get the effective moduli is to apply a displacement field corresponding to uniform elastic strains on the boundary of the RVE, apply the finite element method to calculate the stress field inside the RVE and then get the average stress. Since the average stress is equal to the product of an effective elasticity matrix and the average strain, the effective mouduli can be thereafter identified from the elasticity matrix. Fig. 5 and Fig. 6 show the variations of effective bulk and shear moduli of the nanoporous material with the radius of the circular void, respectively. The present numerical results correspond to a volume fraction of 0.3, i.e. the ratio of the volume of nanovoids to the total volume is 30%. Both the bulk and the shear moduli show size-dependency. For nanoporous material with Type A surface, whose surface Young's modulus E^s is negative (= -7.9253 N/m), the bulk and the shear moduli are increasing as the void size increases. On the contrary, for Type B surface whose Young's modulus E^s is positive (=5.1882 N/m), the effective moduli are decreasing with increasing void size. For a nanoporous material containing nanovoids with their radii in the range of hundred nanometers, its effective mouduli are essentially closed to those without the consideration of the surface effects.

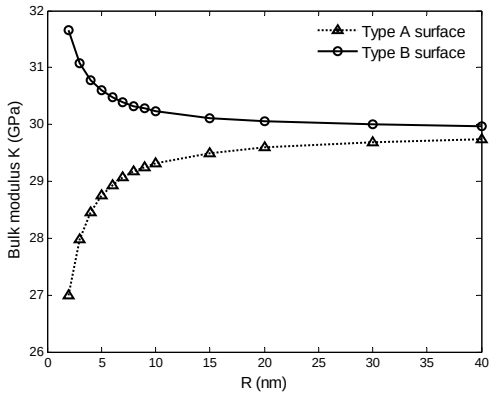

Fig. 5 Varation of effective bulk modulus with the radius of nanovoid

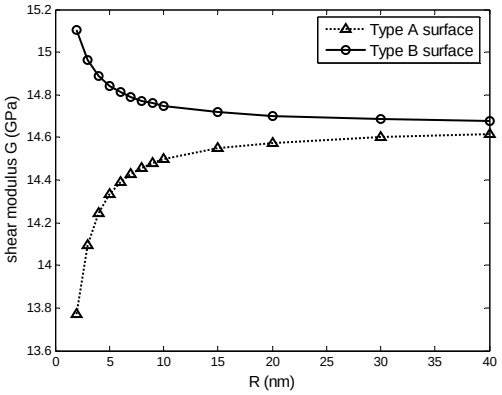

Fig. 6 Varation of effective shear modulus with the radius of nanovoid

V. Conclusion

A finite element approach is proposed in this study to investigate the effects of surface/interface stress on nanoscale structures. Truss element is used to calculate of the contributions of surface/interface to the total potential energy of a nanosystem, and the Gurtin and Murdoch surface/interface stress model is implemented through a user subroutine called 'usermat.f', which is compiled and linked with the general finite element code ANSYS through its User Programmable Features (UPF). The size-dependent stress concentration around a nanoscale circular hole in an infinite material plane is investigated. It is noted that if the surface elastic modulus is positive, the stress concentration is reduced compared with the classical elastic solution, while it is increased for a hole with negative surface modulus. The effective elastic moduli of an elastic solid containing nanoscale circular voids is shown to be size-dependent. Depending on the nature of the surface (i.e. with positive or negative surface modulus), the bulk and shear moduli of a nanoporous material may increase or decrease toward to the convention results without the consideration of the surface effects, as the radii of nanovoids within the solid increase. The present modeling approach can be readily extended to study the mechanical behaviour of nanomaterials and nanostructures with the bulk material shows nonlinear constitutive behaviour and/or under large deformation.

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REFERENCES

[1] G. Y. Jing, H. L. Duan, X. M. Su, Z. S. Zhang, J. Xu, Y. D. Li, J. X. Wang and D. P. Yu, "Surface effects on elastic properties of silver nanowires: contact atomic-force microscopy," *Physical Review B*, vol.73, pp. 235409(1)-235409(6), 2006.

[2] M. E. Gurtin, and A. I. Murdoch, "A continuum theory of elastic material surfaces," *Arch. Ration. Mech. Anal.*, vol. 57, pp. 291-323, 1975.

[3] M. E. Gurtin, and A. I. Murdoch, "Surface stress in solids," *Int. J. Solids and Struct.*, vol.14, pp. 431-440, 1978.

[4] R. E. Miller, and V. Shenoy, "Size-dependent elastic properties of nanosized structural elements," *Nanotechnology*, vol. 11, pp. 139-147, 2002.

[5] P. Sharma, S. Ganti, and N. Bhate, "Effect of surfaces on the size-dependent elastic state of nano-imhomogeneities," *Applied Physics Letters*, vol. 82, pp.535-537, 2003.

[6] 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.

[7] F. Yang, "Size-dependent effective modulus of elastic composite materials: spherical nanocavities at dilute concentrations," *J. Applied Physics*, vol. 95, pp. 3516-3520, 2004.

[8] G. F. Wang, and T. J. Wang, "Deformation around a nanosized elliptical hole with surface effect," *Applied Physics Letter*s, vol. 89: pp. 161901-161903, 2006.

[9] 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.

[10] L. Tian L, and R. K. N. D. Rajapakse, "Elastic field of an isotropic matrix with a nanoscale elliptical imhomogeneity," *Int. J. Solids Struct.*, vol. 44, pp. 7988-8005, 2007.

[11] H. L. Duan, J. Wang, Z. P. Huang, and B. L. Karihaloo, "Size-dependent effective elastic constants of solids containing nano-imhomogeneities 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] ANYSY INC, *Documentation for ANSYS*, Release 10.0, 2006.