Finite element based micromechanical model for elastic materials containing nanoscale inhomogeneities

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Abstract

Nano-structured materials (e.g. nanocomposites, nanoporous materials, nanocrystalline materials, etc.) and nano-scale structural elements (e.g. nanotubes, nanofilms, nanobeams, etc.) have unique mechanical and physical properties. For nano-structured materials containing inhomogeneities (e.g. voids and particles) in the nanoscale dimensions such as nanoporous materials and nanocomposites, the size effect due to surface energy due to nanoscale inhomogeneities can play an important role on their mechanical properties and responses. In this paper, the finite element based micromechanical model for analysis of materials containing nanoscale inhomogeneities incorporating Gurtin-Murdoch surface theory is presented. The proposed micromechanical model is applied to examine the responses and properties of nano-structured materials, i.e., nanoporous and nanocomposite materials. Selected numerical results are presented to portray the features of the elastic field responses and properties of elastic materials with nanoscale inhomogeneities. The finite element-based micromechanical model presented in this paper is an efficient tool to analyze the response and predict the mechanical properties of nano-structured materials.

Keywords: Nanotechnology, micromechanics theory, inhomogeneity, nanocomposites, nanoporous materials

Introduction

Nanomechanics is a study of responses and properties of materials and structures at the nanoscale. Steritz et al. [1] and Dingreville et al. [2] have clearly explained that atoms adjacent to the free surface have a different local environment than do atoms in the bulk of a material. The nanoscale materials or structures contain larger fraction of energy associated with surface atoms when compared to those in the bulk material, and as a result, structures at the nanoscale are known to exhibit size-dependent behavior.

Within the context of modelling nanoscale behavior of materials and structures, two predominant mathematical approaches have been commonly employed in the literature, one known as the molecular or atomistic simulations and the other corresponding to the modified continuum-based models. The molecular-based models, while providing more direct response prediction, generally consume tremendous computational resources because billions of atoms at the nanoscale is needed to include in the simulation models. The continuum-based models, in contrast to the molecular-based models, are less complicated and much more computationally efficient.

Gurtin-Murdoch model, proposed by Gurtin and Murdoch [3, 4], is a mathematical model that incorporates the effects of surface and interfacial energy into continuum mechanics. A good agreement between solutions based on the Gurtin–Murdoch model and atomistic simulations for nano-scale structures has been reported by various researchers (e.g., [5-7]). Sapsathiarn and Rajapakse [7] shown that the Gurtin-Murdoch nanoscale beam model is capable of simulating the experimental results of chromium cantilever beams loaded by an atomic force microscope. Mogilevskaya et al. [8] considered the multiple interaction of circular nano-inclusions in unbounded domain by using a complex variables formulation. Fang et al. [9] studied the elastic interaction between screw dislocations and an embedded coated circular nanowire with interface stresses based on Gurtin and Murdoch theory and explained that the effect of the interface stress on the motion and the equilibrium position of the dislocation near the nanowire is significant when the radius of the nanowire is reduced to nanometer dimensions. A finite-element formulation for static and dynamic modeling of circular nanoplates based on Gurtin-Murdoch theory has been presented by Sapsathiarn and Rajapakse [10]. Mi and Kouris [11] examined the stress concentration Stress concentration in the vicinity of a nanovoid near the free surface of an elastic half-space and its dependence on surface properties.

In this paper, a finite element based micromechanical model for elastic materials with nanoscale inhomogeneities incorporating Gurtin-Murdoch surface stress effects is developed. Selected numerical results for the elastic fields and properties of elastic composites containing nanoscale inhomogeneities, i.e., nanoporous and nanocomposite materials, are presented. The finite element-based micromechanical model of nanoparticle-reinforced composites developed in the present study is an efficient tool to investigate the response and properties of nano-structured materials with practically useful arbitrary shaped nanoscale inhomogeneities, multiple voids/particles, non-symmetric loading, etc.

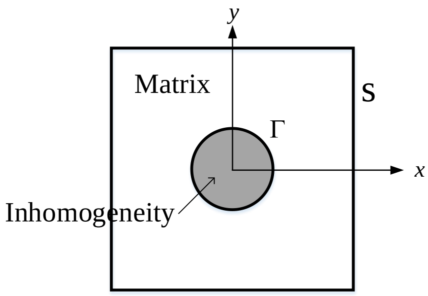


Figure 1. A representative volume element for composite materials containing a nanoscale inhomogeneity, e.g., nanovoid or nanoparticle.

Theoretical consideration

Consider a two-dimensional material plane containing a nanoscale inhomogeneity, e.g., nanovoid or nanoparticle, as shown in Fig. 1. In the case of material with a nanoparticle, the matrix and inhomogeneity are considered as linearly orthotropic materials and the matrix-inhomogeneity bonding is assumed to be perfect. The Cartesian coordinates (x,y) is used in the formulation. The research methodology, procedures and fundamental theories to be employed in the analysis are summarized in the subsequent sections.

Governing equations and surface elasticity model

Regarding linear elasticity theory, the equilibrium equation in the absence of body forces and the constitutive relation of the bulk material can be written using the standard indicial notation as

$$\sigma^B_{ij,j} = 0; \; \sigma^B_{kl} = C_{ijkl}\varepsilon_{ij} \qquad (1)$$

where $\sigma^B_{ij,j}$ denotes the components of stress tensor for a bulk material (inhomogeneity and matrix); ε_{ij} and σ^B_{kl} denote the second-rank tensors of strain and stress respectively; and the elastic matrix C_{ijkl} is the fourth-rank tensor.

The elastic matrices **D** in the Voigt notation for plane stress and plane strain deformations can be written as

$$\mathbf{D} = \left[C_{ijkl}\right] = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{bmatrix} ; \quad \mathbf{D} = \begin{bmatrix} C_{11} - (D_{13}{}^2 / C_{33}) & C_{12} - (C_{13}C_{23} / C_{33}) & 0 \\ C_{12} - (C_{13}C_{23} / C_{33}) & C_{22} - (C_{23}{}^2 / C_{33}) & 0 \\ 0 & 0 & C_{66} \end{bmatrix} \tag{2}$$

(plane stress) (plane strain)

where C_{ij} is the component of elastic compliance matrix in the Voigt notation.

The incorporation of surface stress effects is needed due to the fact that the inhomogeneity in the composite is in a nanoscale size. Gurtin and Murdoch [3, 4] proposed a surface stress model to account for the surface effects at the nanoscale. Models of nanoscale structures based on the Gurtin-Murdoch continuum theory have an elastic surface, mathematically zero thickness, perfectly bonded to the bulk material. The elastic surface has distinct material properties and accounts for the surface energy effects [6]. The generalized Young-Laplace equation [12], surface constitutive relations and strain-displacement relationship of the surface can be expressed as [3, 4]

$$\sigma^s_{\beta\alpha,\beta} + \langle \sigma^B_{\beta\alpha} n_\beta \rangle = 0; \; \langle \sigma^B_{ji} n_i n_j \rangle = \sigma^s_{\beta\alpha} k_{\beta\alpha} \tag{3a}$$

$$\sigma^s_{\beta\alpha} = \tau_0 \delta_{\beta\alpha} + 2 \;\; \mu^S - \tau_0 \;\; \varepsilon_{\beta\alpha} + \;\; \lambda^S + \tau_0 \;\; \varepsilon_{\gamma\gamma} \delta_{\beta\alpha} + \tau_0 u^s_{\beta,\alpha} \tag{3b}$$

$$\varepsilon^s_{\alpha\beta} = \frac{1}{2} \;\; u^s_{\alpha,\beta} + u^s_{\beta,\alpha} \tag{3c}$$

where superscripts *B* and *S* denote the quantities corresponding to the bulk and the surface respectively; $\langle * \rangle = (*)_M - (*)_I$ denotes the jump of the field quantity across the inhomogeneity and matrix interface where the subscripts *M* and *I* are used to identify quantities associated with the matrix and the inhomogeneity respectively; μ^S and λ^S are surface Lamé constants; τ_0 is the residual surface tension under unstrained conditions; n_i denotes the components of the unit normal vector of the surface; and $k_{\beta\alpha}$ is the curvature tensor of the surface. It should be noted that the surface material properties, μ^S, λ^S and τ_0 can be determined from atomistic simulations [13].

Tian and Rajapakse [14] presented a finite element formulation for the analysis of a two-dimensional elastic material plane containing a nanoscale inhomogeneity by employing the energy method. The potential energy ($\prod$) of the system in Fig. 1 consists of the elastic strain energies of the bulk inhomogeneity (U^{BI}) and matrix (U^{BM}) materials, the surface elastic strain energy (U^S) due to the surface effects and the potential energy (*W*) due to the application of external loads, and can be written as

$$\prod = U^{BI} + U^{BM} + U^S + W \tag{4}$$

in which the superscript *BI* and *BM* denotes quantities corresponding to the bulk inhomogeneity and matrix materials respectively.

The elastic strain energies for the bulk inhomogeneity (U^{BI}) and for the matrix material (U^{BM}) can be expressed as

$$U^{BI} = \int_{V_I} \int_0^{\varepsilon_{ij}} \sigma_{ij}^B d\varepsilon_{ij} dV \, ; \, U^{BM} = \int_{V_M} \int_0^{\varepsilon_{ij}} \sigma_{ij}^B d\varepsilon_{ij} dV \tag{5}$$

The potential energy (*W*) due to the application of external loads can be expressed as

$$W = -\int_{V_I} \{u\}^{\mathrm{T}} \{T\} dS \tag{6}$$

where T and u denote the vectors of surface traction and surface displacement respectively; and the superscript T denotes the transpose of a vector or matrix.

Based on the Gurtin-Murdoch surface stress model expressed in Eq. (3), the surface elastic strain energy (U^S) can be obtained as

$$U^S = \int_{\Gamma+S} \int_0^{\varepsilon_{\alpha\beta}} \sigma_{\alpha\beta}^S d\varepsilon_{\alpha\beta} d\Gamma \tag{7}$$

Introducing the element shape function $N(x,y)$ to interpolate the field variables u within an element by

$$\{u\} = [N]\{\bar{u}\} \tag{8}$$

where u denotes nodal displacement vector.

The element strain vector {ε} can be determined from Eq. (8) using the classical strain-displacement relation as

$$\{\varepsilon\} = [B]\{\bar{u}\} \tag{9}$$

where $[B]$ is a strain-displacement matrix in which the elements are the derivatives of the element shape functions, $[B] = \partial[N]/\partial x_i$.

Substitution of Eq. (8) and (9) into Eq. (5) - (7) together with the constitutive relations for bulk (matrix and inhomogeneity) and surface materials, Eq. (4) becomes

$$\begin{aligned} \prod = & \int_{V_M} \frac{1}{2}\{\bar{u}\}^{\mathrm{T}}[B]^{\mathrm{T}}[D]_M[B]\{\bar{u}\}dV + \int_{V_I} \frac{1}{2}\{\bar{u}\}^{\mathrm{T}}[B]^{\mathrm{T}}[D]_I[B]\{\bar{u}\}dV \\ & -\int_S [N]\{\bar{u}\}^{\mathrm{T}}\{T\}dS + \int_{\Gamma+S} \frac{1}{2}\{\bar{u}\}^{\mathrm{T}}[B]^{\mathrm{T}}[D]_S[B]\{\bar{u}\}d\Gamma \end{aligned} \tag{10}$$

Applying the stationary condition of $\prod$, i.e., $\delta\prod = 0$, with respect to the nodal displacement components, the equilibrium equations for system in Fig. 1 can be obtained as

$$[K]\{\bar{u}\}=\{f\} \tag{11}$$

where

$$[K]=\int_{V_M}[B]^{\mathrm{T}}[D]_M[B]dV+\int_{V_I}[B]^{\mathrm{T}}[D]_I[B]dV+\int_{\Gamma+S}[B]^{\mathrm{T}}[D]_S[B]d\Gamma \quad (12a)$$

$$\{f\}=\int_S[N]\{T\}dS \quad f = \int_S N \quad T \quad dS \quad (12b)$$

Micromechanical model of nanocomposites

A micromechanical model based on finite element formulation given in the preceding section is developed in the present study for analysis of elastic materials containing nanoscale inhomogeneities. The micromechanical analysis is performed by using a micromechanics theory which relates mechanics between two different length scale problems, i.e., (1) the macroscopic level in which the material is conceptually represented as a homogeneous material and (2) the level of the constituents in which the material properties are always heterogeneous and consist of distinguishable phases such as the main matrix material, inclusions and cavities or voids. Properties of elastic materials containing nanoscale inhomogeneities can be determined by the analysis in the level of the constituents. The analysis might be performed on a "representative volume element" or a "unit cell" which can be isolated from the composite material and is in a state of equilibrium. The unit cell for materials considered in the present work is schematically presented in Fig. 1.

The macroscopic constitutive relation of the materials with nanoscale inhomogeneities can be expressed in terms of the macro stress and the macro strain as

$$\{\bar{\sigma}\}=\left[C^{eff}\right]\{\bar{\varepsilon}\} \quad (13)$$

where

$$\{\bar{\sigma}\}=\begin{bmatrix}\bar{\sigma}_{xx} & \bar{\sigma}_{yy} & \bar{\sigma}_{xy}\end{bmatrix}^{\mathrm{T}};\ \{\bar{\varepsilon}\}=\begin{bmatrix}\bar{\varepsilon}_{xx} & \bar{\varepsilon}_{yy} & \bar{\varepsilon}_{xy}\end{bmatrix}^{\mathrm{T}} \quad (14a)$$

$$\left[C^{eff}\right]=\begin{bmatrix}C_{11}^{eff} & C_{12}^{eff} & 0\\ C_{12}^{eff} & C_{22}^{eff} & 0\\ 0 & 0 & C_{66}^{eff}\end{bmatrix} \quad (14b)$$

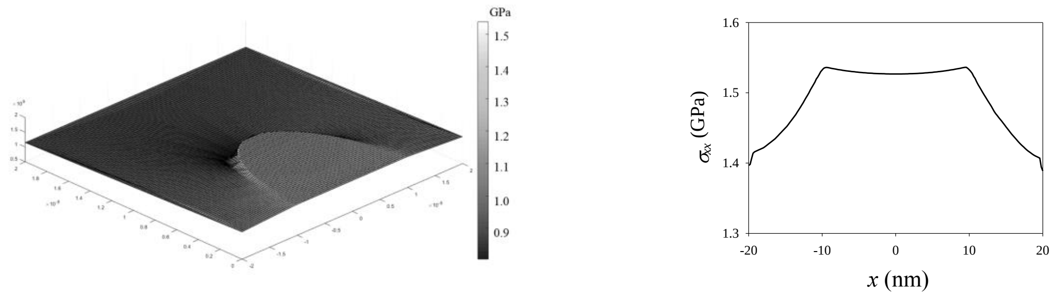
According to the micromechanics theory, the macro stress, $\bar{\sigma}_{ij}$, and macro strain, $\bar{\varepsilon}_{ij}$, can be defined as the volume average stress in a RVE as

$$\bar{\sigma}_{ij}=\frac{1}{V}\int_{\Omega}\sigma_{ij}\,d\Omega;\ \ \bar{\varepsilon}_{ij}=\frac{1}{V}\int_{\Omega}\varepsilon_{ij}\,d\Omega \quad (15)$$

Numerical results and discussion

A selected set of numerical solutions is presented in this section for the plane strain case of elastic material with nanoscale inhomogeneity to portray the response within nano-structured materials and investigate the influence of inhomogeneity volume fraction to the mechanical properties of the nano-structured materials. Two types of materials are considered in the numerical simulation, i.e. (1) nanocomposite materials (i.e., materials containing nanoscale particles) and (2) nanoporous materials (i.e., materials containing nanoscale cavities or voids). The matrix and particle inhomogeneity materials are considered to be linearly elastic and isotropic in the numerical study with Lame′ constants, E_M = 40 GPa, v_M = 0.20 GPa for the matrix material and E_I = 80 GPa, v_I = 0.25 GPa for the particle inhomogeneity material. The surface parameter $K^S = 2\mu^S + \lambda^S - \tau_0 = 10$ N/m is considered in the numerical example.

The unit cell subjected to a prescribed displacement in the *x*-direction over the positive *x* face (a surface that is perpendicular to the *x*-axis and on the positive *x* side) is considered in the numerical example. The other faces are constrained in such a way that only the movement in the *x*-direction is allowed and the displacements in all other directions are prevented. The properties of nanocomposite and nanoporous materials can be determined from the fields within the unit cell being considered by using Eqs. (13)-(15).



(a) σ_{xx} distribution (b) σ_{xx} profile (across the inhomogeneity)

Figure 2. (a) Distribution and (b) profile of the stress σ_{xx} for nanocomposites with circular nano-particles

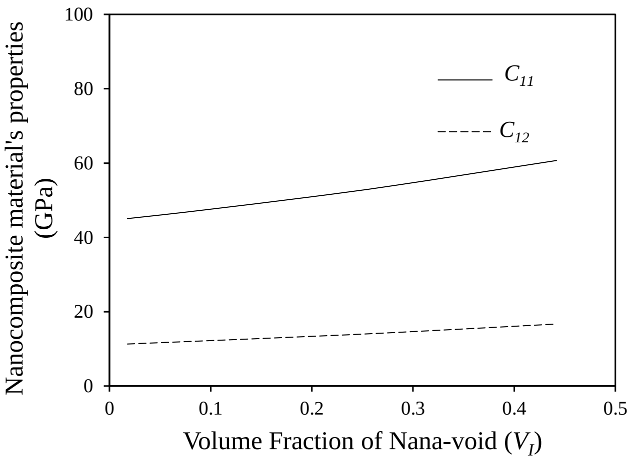


Figure 3. Variation of material properties of nanocomposites with circular nano-particles versus the volume fraction of the inhomogeneity (V_I).

The numerical results for the case of nanocomposites containing circular nano-particles are presented in Figs. 2 and 3. The distribution of stress σ_{xx} over the half-domain of the unit cell is presented in Fig. 2(a) for a nanocomposite material with volume fraction of the inhomogeneity V_I = 0.2. The corresponding profile of stress σ_{xx} along the *x*-axis across the center of the nano-particle inhomogeneity is presented in Fig. 2(b). The unit cell is stretched and the tensile stress σ_{xx} is generated all over the unit cell. The stress σ_{xx} in the domain of inhomogeneity is generally higher compared to those in the matrix domain showing the stress disturbance in a composite material due to the presence of the nanoscale inhomogeneity. The influence of volume fraction of the inhomogeneity (V_I) to the mechanical properties C_{11}^{eff} and C_{12}^{eff} of the nanocomposite can be observed in Fig. 3. It is shown in Fig. 3 that the properties of nanoinclusion material are increasing as the volume fraction V_I increases. It should be observed that the relations between the material coefficients and V_I are non-linear.

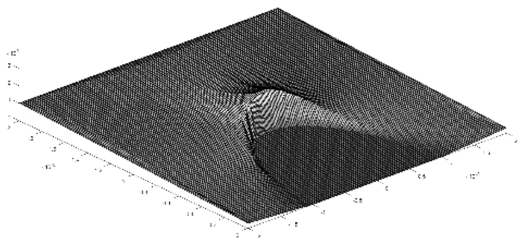


Figure 4. Distribution of the stress σ_{xx} for nanoporous material's properties with circular nano-voids.

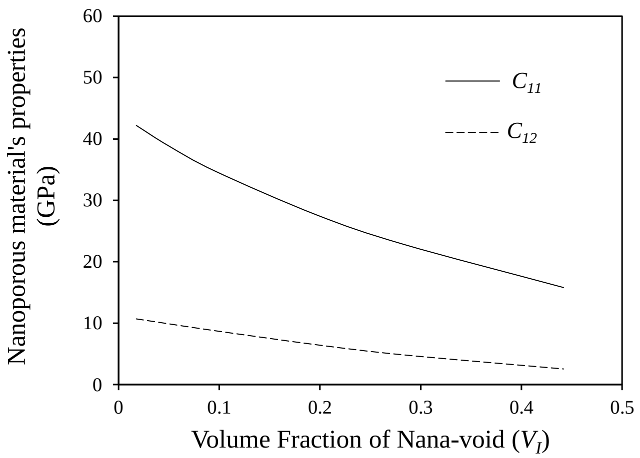


Figure 5. Variation of nanoporous material's properties (circular nano-voids) versus the volume fraction of the inhomogeneity (V_I).

The stress distribution and properties of nanoporous material with circular nano-voids considered in the numerical study are presented in Figs. 4 and 5 respectively. The volume fraction of the inhomogeneity (nanoscale voids) considered in Fig. 4 is V_I = 0.2. Similar behavior is observed for the case of a nanoporous material, i.e., the unit cell is stretched and the tensile stress σ_{xx} is generated all over the domain. Based on the results shown in Fig. 4, the stress concentration in the vicinity of a nanovoid is noted. Similar to the case of nanocomposite, the dependence of nanoporous material's properties on the volume fraction of the inhomogeneity (*VI*) is non-linear (see Figs. 3 and 5). As expected, the properties of nanoporous material are decreasing as the volume fraction of nanovoid V_I increases.

Conclusions

In this paper, a finite element-based micromechanics model for analysis of elastic materials containing nanoscale inhomogeneities incorporating surface stress effects has been developed. The Gurtin-Murdoch surface elasticity is employed in the micromechanical model to incorporate the interface energy effects of nanoscale inhomogeneity. Selected numerical results are presented to portray the features of the elastic field responses and properties of elastic materials with nanoscale inhomogeneities. Two types of materials are considered in the numerical simulation, i.e. nanocomposite materials (i.e., materials containing nanoscale particles) and nanoporous materials (i.e., materials containing nanoscale cavities or voids). Numerical results of stress and material properties for nanocomposite and nanoporous materials show considerable dependence on volume fraction of inhomogeneity. The finite element-based micromechanical model provides an efficient tool to analyze and predict the mechanical response of nano-inhomogeneities with arbitrary-shaped nanoscale particles, multiple particles, nanovoid, multiple nanovoid, non-symmetric loading, etc.

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