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Boundary element analysis of nanoinhomogeneities of arbitrary shapes with surface and interface effects

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ABSTRACT

In this paper, a boundary element method (BEM) is proposed to analyze the stress field in nanoinhomogeneities with surface/interface effect. To consider this effect, the continuity conditions along the internal interfaces between the matrix and inhomogeneities are modeled by the well-known Gurtin–Murdoch constitutive relation. In the numerical analysis, the interface elastic moduli and the geometry of the nanoscale inhomogeneity are varied to show their influence on the induced stress field. The interaction between nanoscale inhomogeneities and the effect of different geometric shapes of inhomogeneities, including ellipse, triangle, and square are also investigated for different interfacial energy and geometry of nanoscale inhomogeneities. The proposed BEM formulation is very general, including the complete Gurtin–Murdoch model and is further convenient for arbitrary shapes of inhomogeneity. © 2011 Elsevier Ltd. All rights reserved.

1. Introduction

Nanocomposites have been widely applied to the microelectromechanical system, bioengineering, and optics/photonics devices due to their unique mechanical, electronic, and optical properties [1–4]. Unlike bulk materials, the effective elastic properties of nanomaterials strongly depend on the material and geometric parameters of the nanostructure as well as on the interface diffusion between the nanoinhomogeneity and matrix. While the surface/interface stresses of the nanostructure can be determined either experimentally [5,6] or computationally [7,8], its sizedependent properties can be explained by considering the effect of the surface/interface stresses, which comes from the excess free energy along the surface/interface (e.g., Refs. [9,10]).

A linearized stress-strain constitutive relation in surface elasticity was proposed by Gurtin and Murdoch [11], Murdoch [12], and Gurtin et al. [13]. This so-called Gurtin–Murdoch model has become increasingly popular and is now widely applied to investigate the mechanical behavior of nanoscale inhomogeneities. For instance, the size-dependent problem of the mechanical behavior of nanoscale inhomogeneities, Eshelby's tensor for embedded nanoinclusions, and the effective elastic constants of nanoscale inhomogeneities have been studied using the Gurtin– Murdoch model [10,14,15].

A couple of other recent studies represent the increasing interests in this direction: He and Li [16] considered the effect of the surface stress on the stress concentration near a spherical void in an elastic medium using the Papkovitch-Neuber displacement potential and Gurtin-Murdoch model. Also using the Gurtin-Murdoch model, Lim et al. [17] studied the influence of the interfacial stress on the elastic field in an infinite solid containing a nanoscale spherical inclusion with an axisymmetric eigenstrain. Tian and Rajapakse [18,19] presented analytical solutions for a single circular/elliptical nanoinhomogeneity embedded in an infinite isotropic elastic matrix. The corresponding finite-element method was also introduced to analyze the effect of surface and interfacial energy on the field quantities [20,21]. By incorporating surface/interface tension, Sharma and Wheeler [22] investigated the size-dependent elastic field of an ellipsoidal nanoinclusion under a pure dilatation eigenstrain. Ou et al. [23] discussed the effect of the residual surface tension on the stress concentration around a nanoscale spheroidal cavity under arbitrary uniform remote loadings. Luo and Wang [24] studied the anti-plane elastic field of an infinite matrix containing a nanoscale elliptical inhomogeneity.

In most of the works cited above, the simplified Gurtin– Murdoch stress–strain constitutive relation was used where the whole or part of the displacement–gradient term was neglected [25,26]. Using the complex variable method, Mogilevskaya et al. [27] recently studied the multiple interactions between the circular nanoinhomogeneities and nanopores using the "complete" Gurtin–Murdoch model. In their formulation, the precise component form of the three-dimensional Gurtin–Murdoch

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equation for the interface between the matrix and an arbitrarily shaped inhomogeneity was employed.

This paper studies the mechanical behavior of nanoscale inhomogeneities with surface and interface effect. The boundary element method (BEM) is introduced to handle the problem, and the precise component form of the Gurtin-Murdoch constitutive relation along the surfaces/interfaces is employed. The proposed numerical algorithm requires only discretization on the interfaces between the nanoinhomogeneities and matrix, and can be further applied easily to the inhomogeneities of arbitrary shape. The paper is organized as follows. In Section 2, the problem is described with the basic integral equations being introduced. In Section 3, the boundary element formulations for the matrix and nanoinhomogeneities are presented along with their continuity conditions on the interfaces. In Section 4, the effect of the surface/ interface parameters, the shape and size of the nanoinhomogeneities on the stress field is investigated in details. A summary of the present work is given in Section 5.

2. Problem description and basic integral equations

2.1. Problem description

We consider the plane–strain problem where an elastic isotropic infinite matrix is subjected to a remote stress field. The matrix contains a total of *K* nanocavities and/or nanoinhomogeneities of arbitrary shape. The *k*-th surface of the nanocavity or the *k*-th interface between the nanoinhomogeneity and matrix is denoted by Γ_k (k=1 to K), which will be also called boundary Γ_k hereafter. All the surfaces and/or interfaces (or boundaries) follow the Gurtin–Murdoch constitutive relation.

2.2. Boundary integral equations of the matrix

The displacement integral equations at point *P* within the matrix can be given as follows [28] (for $\alpha = 1,2$):

$$u_{\alpha}(P) = u_{\alpha}^{0}(P) + \sum_{k=1}^{K} \int_{\Gamma_{k}} U_{\alpha\beta}(P,q_{k}) t_{\beta}^{k}(q_{k}) d\Gamma(q_{k})$$
$$- \sum_{k=1}^{K} \int_{\Gamma_{k}} T_{\alpha\beta}(P,q_{k}) u_{\beta}^{k}(q_{k}) d\Gamma(q_{k})$$
(1)

where q_k is the field point on the *k*-th boundary Γ_k . u_k^k and t_β^k are, respectively, the displacements and tractions on Γ_k . u_{α}^0 (α =1, 2) are the displacements at point *P* related to the remote stress field in an infinite homogeneous matrix. $U_{\alpha\beta}$ and $T_{\alpha\beta}$ are the fundamental displacement and traction solutions in the corresponding elastic isotropic infinite plane [29].

We now let the internal point *P* approach point p_k on the *k*-th boundary Γ_k . Then Eq. (1) becomes

$$\begin{aligned} c_{\alpha\beta}^{k}u_{\beta}(p_{k}) &= u_{\alpha}^{0}(p_{k}) + \sum_{i=1}^{K} \int_{\Gamma_{i}} U_{\alpha\beta}(p_{k},q_{i})t_{\beta}(q_{i})d\Gamma \\ &- \sum_{i=1, \neq k}^{K} \int_{\Gamma_{i}} T_{\alpha\beta}(p_{k},q_{i})u_{\beta}(q_{i})d\Gamma - \int_{\Gamma_{k}}^{c} T_{\alpha\beta}(p_{k},q_{k})u_{\beta}(q_{k})d\Gamma \end{aligned}$$

$$(2)$$

where $c_{\alpha\beta}^k$ depends on the geometry at the boundary point p_k . The symbol \int^c denotes the Cauchy principal integral.

2.3. Boundary integral equations of the inhomogeneity

If the *k*-th boundary is an interface between the matrix and nanoinhomogeneity, we will then also need the boundary integral equation on the interface from the inhomogeneity side. Therefore

on the *k*-th interface from the inhomogeneity side, the corresponding displacement boundary integral equation can be given as [29]

$$c_{\alpha\beta}^{k}(p)u_{\beta}^{k}(p) = \int_{\Gamma_{k}} U_{\alpha\beta}^{k}(p,q)t_{\beta}^{k}(q)d\Gamma(q) - \int_{\Gamma_{k}}^{c} T_{\alpha\beta}^{k}(p,q)u_{\beta}^{k}(q)d\Gamma(q)$$
(3)

The notations used in Eq. (3) bear the same physical meanings as those in Eq. (2). The only difference is that in Eq. (3), a superscript k is added to the fundamental displacement and traction solutions to emphasize that these solutions are associated with the k-th inhomogeneity.

2.4. Continuity conditions along the interface between the matrix and inhomogeneity

Along the *k*-th surface/interface, the Gurtin–Murdoch model will be followed [30]. These conditions are discussed below.

(a) Continuity of displacements (on the *k*-th interface in terms of the Cartesian (*x*,*y*)-components)

$$u_{kx}^{inh} = u_{kx}^{mat} = u_{kx}, \quad u_{ky}^{inh} = u_{ky}^{mat} = u_{ky}$$
(4)

where the superscripts *inh* and *mat* indicate the elastic fields on the interface from the inhomogeneity and matrix side, respectively. Eq. (4) is required only if one deals with an interface.

(b) Interface equilibrium conditions (on the *k*-th interface in terms of the normal and tangential (*n*,*l*)-components of the interface) [30]

$$\sigma_{kl}^{inh} - \sigma_{kl}^{mat} = \frac{\partial \sigma_k^{sur}}{\partial s} + \frac{\sigma_{k0} \omega_k^{sur}}{\rho_k}$$
$$\sigma_{kn}^{inh} - \sigma_{kn}^{mat} = -\frac{\sigma_k^{sur}}{\rho_k} + \sigma_{k0} \frac{\partial \omega_k^{sur}}{\partial s}$$
(5)

where *s* is the arc length of the undeformed interface. It should be pointed out that in the above equations, if the *k*-th boundary is the surface of a nanocavity, then σ_{kl}^{inh} and σ_{kn}^{inh} equal zero. Also in Eq. (5), σ_{k0} and ρ_k are, respectively, the residual interface tension on, and the curvature radius of, the *k*-th interface. The subscripts *l* and *n* indicate the unit tangential direction (counterclockwise) and unit outward normal direction along the nanoinhomogeneity boundary Γ_k . σ_k^{sur} is the surface/interface stress, which will be further discussed below, and

$$\omega_k^{\text{sur}} = -\frac{u_{kl}}{\rho_k} + \frac{\partial u_{kn}}{\partial s} \tag{6}$$

where u_{kl} , u_{kn} are the tangential and normal components of the displacement in the local (n,l)-coordinate system.

(c) Constitutive equation for the surface/interface The surface/interface stress σ_k^{sur} on the *k*-th boundary can be related to the surface/interface strain ε_k^{sur} as

$$\sigma_k^{sur} = \sigma_{k0} + (2\mu_{k0} + \lambda_{k0})\varepsilon_k^{sur} \tag{7}$$

where μ_{k0} , λ_{k0} are the Lame constants on the *k*-th surface/ interface, and the strain ε_k^{sur} can be further related to the local (n,l)-displacement components via the following form:

$$\varepsilon_k^{\text{sur}} = \frac{u_{kn}}{\rho_k} + \frac{\partial u_{kl}}{\partial s} \tag{8}$$

3. Boundary element formulations

3.1. Boundary element formulation of the matrix

Three nodal quadratic elements are adopted to discretize Eq. (2) on the matrix side. The discretized version of Eq. (2) can

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be written as

$$\begin{bmatrix} \boldsymbol{h}_{1}^{\text{mat}} & \boldsymbol{h}_{2}^{\text{mat}} & \cdots & \boldsymbol{h}_{K}^{\text{mat}} \end{bmatrix} \begin{cases} \boldsymbol{u}_{1}^{\text{mat}} \\ \boldsymbol{u}_{2}^{\text{mat}} \\ \vdots \\ \boldsymbol{u}_{K}^{\text{mat}} \end{cases} \\ = \begin{bmatrix} \boldsymbol{g}_{1}^{\text{mat}} & \boldsymbol{g}_{2}^{\text{mat}} & \cdots & \boldsymbol{g}_{K}^{\text{mat}} \end{bmatrix} \begin{cases} \boldsymbol{t}_{1}^{\text{mat}} \\ \boldsymbol{t}_{2}^{\text{mat}} \\ \vdots \\ \boldsymbol{t}_{K}^{\text{mat}} \end{cases} + \begin{cases} \boldsymbol{f}_{1}^{0} \\ \boldsymbol{f}_{2}^{0} \\ \vdots \\ \boldsymbol{f}_{K}^{0} \end{cases}$$
(9a)

where \boldsymbol{u}_k and \boldsymbol{t}_k are the nodal displacement and traction matrices on the *k*-th boundary (from the matrix side); \boldsymbol{h}_k and \boldsymbol{g}_k are the influence matrices on the *k*-th boundary associated, respectively, to the fundamental displacement and traction solutions \boldsymbol{U} and \boldsymbol{T} (in the matrix); \boldsymbol{f}_k^0 is a known vector associated with the homogeneous displacement field \boldsymbol{u}_k^0 in Eq. (2).

Equation (9a) can be simply expressed in a condensed matrix form as follows:

$$\boldsymbol{h}_m \boldsymbol{u}_m = \boldsymbol{g}_m \boldsymbol{t}_m + \boldsymbol{f}^0 \tag{9b}$$

where

$$\boldsymbol{h}_{m} = \begin{bmatrix} \boldsymbol{h}_{1}^{\text{mat}} & \boldsymbol{h}_{2}^{\text{mat}} & \cdots & \boldsymbol{h}_{K}^{\text{mat}} \end{bmatrix}, \quad \boldsymbol{g}_{m} = \begin{bmatrix} \boldsymbol{g}_{1}^{\text{mat}} & \boldsymbol{g}_{2}^{\text{mat}} & \cdots & \boldsymbol{g}_{K}^{\text{mat}} \end{bmatrix}, \\ \boldsymbol{u}_{m} = \begin{bmatrix} \boldsymbol{u}_{1}^{\text{mat}} & \boldsymbol{u}_{2}^{\text{mat}} & \cdots & \boldsymbol{u}_{K}^{\text{mat}} \end{bmatrix}^{T}, \quad \boldsymbol{t}_{m} = \begin{bmatrix} \boldsymbol{t}_{1}^{\text{mat}} & \boldsymbol{t}_{2}^{\text{mat}} & \cdots & \boldsymbol{t}_{K}^{\text{mat}} \end{bmatrix}^{T} \\ \text{and} \quad \boldsymbol{f}^{0} = \begin{bmatrix} \boldsymbol{f}_{1}^{0} & \boldsymbol{f}_{2}^{0} & \cdots & \boldsymbol{f}_{K}^{0} \end{bmatrix}^{T}. \end{cases}$$

3.2. Boundary element formulation of the inhomogeneity

Similarly, the discretized system corresponding to Eq. (3) can be written as (on the *k*-th interface of the inhomogeneity and matrix, and from the inhomogeneity side)

$$\boldsymbol{h}_{k}^{\mathrm{inh}}\boldsymbol{u}_{k}^{\mathrm{inh}} = \boldsymbol{g}_{k}^{\mathrm{inh}}\boldsymbol{t}_{k}^{\mathrm{inh}} \tag{10a}$$

where the matrices h_k , g_k , u_k , and t_k have the same meanings as in Eq. (9a) but are associated with the *k*-th inhomogeneity.

The condensed matrix form of Eq. (10a) is

$$\boldsymbol{h}_{c}\boldsymbol{u}_{c} = \boldsymbol{g}_{c}\boldsymbol{t}_{c} \tag{10b}$$

where

$$\boldsymbol{h}_{c} = \begin{bmatrix} \boldsymbol{h}_{1}^{\text{inh}} & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{h}_{2}^{\text{inh}} & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{h}_{K}^{\text{inh}} \end{bmatrix}^{T}, \quad \boldsymbol{g}_{c} = \begin{bmatrix} \boldsymbol{g}_{1}^{\text{inh}} & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{g}_{2}^{\text{inh}} & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{g}_{K}^{\text{inh}} \end{bmatrix}^{T},$$
$$\boldsymbol{u}_{c} = \begin{bmatrix} \boldsymbol{u}_{1}^{\text{inh}} & \boldsymbol{u}_{2}^{\text{inh}} & \cdots & \boldsymbol{u}_{K}^{\text{inh}} \end{bmatrix}^{T} \text{ and } \boldsymbol{t}_{c} = \begin{bmatrix} \boldsymbol{t}_{1}^{\text{inh}} & \boldsymbol{t}_{2}^{\text{inh}} & \cdots & \boldsymbol{t}_{K}^{\text{inh}} \end{bmatrix}^{T}$$

3.3. Discretized interface conditions

On the *k*-th boundary (or on the inhomogeneity–matrix interface) Γ_{k} , the following conditions hold. For the displacements, we have

$$\boldsymbol{u}_k^{\text{inh}} = \boldsymbol{u}_k^{\text{mat}} = \boldsymbol{u}_k \quad (k = 1, 2, \dots, K)$$
(11)

For the tractions, we have, for points on the *k*-th nanoinhomogeneity boundary,

$$t_{kx}^{inh} = n_{kx}^{inh} \sigma_{kn}^{inh} - n_{ky}^{inh} \sigma_{kl}^{inh}$$

$$t_{ky}^{inh} = n_{ky}^{inh} \sigma_{kn}^{inh} + n_{kx}^{inh} \sigma_{kl}^{inh}$$
(12a)

and for points on the matrix boundary

$$t_{kx}^{mat} = n_{kx}^{mat} \sigma_{kn}^{mat} - n_{ky}^{mat} \sigma_{kl}^{mat}$$

$$t_{ky}^{mat} = n_{ky}^{mat} \sigma_{kn}^{inh} + n_{kx}^{mat} \sigma_{kl}^{mat}$$
(12b)

where $n_{kx}^{\text{mat}} = -n_{kx}^{\text{inh}}$, $n_{ky}^{\text{mat}} = -n_{ky}^{\text{inh}}$.

From Eq. (12), we have the following relationship:

$$t_{kx}^{inh} + t_{kx}^{mat} = n_{kx}^{inh}(\sigma_{kn}^{inh} - \sigma_{kn}^{mat}) - n_{ky}^{inh}(\sigma_{kl}^{inh} - \sigma_{kl}^{mat})$$
$$t_{ky}^{inh} + t_{ky}^{mat} = n_{ky}^{inh}(\sigma_{kn}^{inh} - \sigma_{kn}^{mat}) + n_{kx}^{inh}(\sigma_{kl}^{inh} - \sigma_{kl}^{mat})$$
(13)

where $\sigma_{kl}^{inh} - \sigma_{kl}^{mat}$ and $\sigma_{kn}^{inh} - \sigma_{kn}^{mat}$ can be evaluated using Eq. (5). Applying Eq. (13) to nodal point $q_{km} \in \Gamma_k$ ($km = 1, 2, \dots, KM$) on the *k*-th interface Γ_k , we have

$$\boldsymbol{t}_{k}^{inh}(q_{km}) + \boldsymbol{t}_{k}^{mat}(q_{km}) = \begin{bmatrix} n_{ky}^{inh}(q_{km}) & -n_{ky}^{ihh}(q_{km}) \\ n_{ky}^{inh}(q_{km}) & n_{kx}^{inh}(q_{km}) \end{bmatrix} \begin{cases} \sigma_{kn}^{inh}(q_{km}) - \sigma_{kn}^{mat}(q_{km}) \\ \sigma_{kl}^{inh}(q_{km}) - \sigma_{kl}^{mat}(q_{km}) \end{cases}$$
(14)

where $\mathbf{t}_k^I = [\mathbf{t}_k^I(q_1) \quad \mathbf{t}_k^I(q_2) \quad \cdots \quad \mathbf{t}_k^I(q_{kM})]^T$ (*I* denotes the inhomogeneity "*inh*" or the matrix "*mat*") are the traction vectors in Eqs. (9) and (10).

From Eq. (14), together with Eqs. (4)–(8), we have

$$\boldsymbol{T}^{inh} + \boldsymbol{T}^{mat} = \mathbf{C}\mathbf{U} + \boldsymbol{F}_0 \tag{15}$$

where **C** is a reduced matrix from Eq. (14) and Eqs. (4)–(8); F_0 is a given vector from the residual stress tension over the interface between the nanoinhomogeneity and matrix.

Based on Eqs. (11) and (14), the final system of equations can be obtained from Eqs. (9b) and (10b) as

(16)

$$AU = F$$

where $A = g_m^{-1} h_m + g_c^{-1} h_c - C$, $F = F_0 + g_m^{-1} f^0$.

Therefore, once Eq. (16) is solved, all the interface displacements can be found. Subsequently, all the interface tractions can



Fig. 1. An infinite plane with a nanosize elliptical hole under a far-field stress.

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be calculated using Eqs. (9b) and (10b). The stress along the circumferential direction of the interface between the nanoinhomogeneity and matrix can be evaluated using the constitutive and

strain-displacement relations. If needed, the stresses at any point within the matrix or nanoinhomogeneity can be calculated using the conventional stress integral equations.



Fig. 2. (a) Stress concentration factor on the surface of the hole at $\theta = 0$ vs. hole size R [=(a+b)/2] and for different interfacial moduli *Ks*. The elliptical ratio is fixed at a/b=1.5 and the matrix is under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$. (b) Oscillation of the stress concentration factor on the surface of the hole at $\theta = 0$ vs. hole size $R [=(a+b)/2] \le 5$ nm and for different interfacial moduli. The elliptical ratio is fixed at a/b=1.5 and the matrix is under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$. (c) Variation of the stress component σ_{xx} along *x*-axis for fixed R = 6 nm (a/b=1.5) and for different interfacial moduli *Ks* under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$. (d) Variation of the stress component σ_{yy} along *x*-axis for fixed R=6 nm (a/b=1.5) and for different interfacial moduli *Ks* under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$. (e) Variation of the stress components σ_{xx} and σ_{yy} along *x*-axis for fixed R=6 nm (a/b=1.5) and for different interfacial moduli stress $\sigma_{yy}^{\infty} = \sigma_0$. (e) Variation of the stress components σ_{xx} and σ_{yy} along *x*-axis for fixed R=6 nm (a/b=1.5) with materials Al [1 0 0] and Al [1 1 1] under residual surface stress σ^0 .

4. Numerical examples

The formulations presented in the previous sections have been programmed and the corresponding code has been validated with existing solutions. For example, for an infinite plane with a circular nanocavity or nanoinhomogeneity under a remote loading, our BEM results are in good agreement with the analytical solutions in Ref. [18]. Also, for both nanocavity and nanoinhomogeneity in an infinite plane under a remote loading, our BEM results are consistent with those in Ref. [27]. Therefore, in what follows, we will analyze a couple of new problems.

4.1. An infinite plane with an elliptical nanocavity

An infinite plane of aluminum with an elliptical hole under the remote loading $\sigma_{yy}^{\infty} = \sigma_0$ is shown in Fig. 1. The bulk material properties of the aluminum are λ_M =58.17 GPa and μ_M =26.13 GPa [31]. The surface elastic constants of the nanocavity are λ^{S} = 3.4939 N/ m, $\mu^{S} = -5.4251$ N/m, $\sigma^{0} = 0.5689$ N/m for Al [100] surface and λ^{S} = 6.8511 N/m, μ^{S} = -0.3760 N/m, and σ^{0} = 0.9108 N/m for Al [1 1 1] surface [7]. We use 32 quadratic elements to discretize the elliptical hole boundary. The surface modulus $Ks (= 2\mu^{S} + \lambda^{S})$ and the nominal radius R (=(a+b)/2) are used to analyze the surface stress effect. Fig. 2a-d shows the variation of different stress components where the residual surface stress σ^0 is assumed to be zero. While Fig. 2a demonstrates that a positive and negative surface modulus Ks would affect the hoop stress in opposite ways [19], Fig. 2b shows that for a negative surface modulus (Ks = -7.92 N/m in this example), the circumferential stress on the hole (say at $\theta = 0$) may even oscillate with varying nominal radius R. This oscillatory behavior was also observed in Ref. [19]. For a/b=1.5 (R=6 nm), the stresses σ_{xx} and σ_{yy} along the x-axis for different Ks are showed, respectively, in Fig. 2c and d, which are similar to the analytical solutions [19]. Fig. 2e shows the distribution of the stresses σ_{xx} and σ_{yy} along the *x*-axis for Al [100] and Al [111] with consideration of the residual surface stress σ^0 , where a/b=1.5 (R=6 nm) and the symbols sxx and syy denote stresses σ_{xx} and σ_{yy} . It is observed from this figure that the induced stress field in the Al [1 1 1] system is larger than that in the Al [1 0 0] system.

4.2. An infinite plane with a nanocavity and a nanoinhomogeneity

An infinite plane containing both nanocavity and nanoinhomogeneity subjected to remote loadings is shown in Fig. 3. The geometry parameters are given as R_1 =5 nm, R_2 =100 nm, and o_1o_2 =107 nm. The elastic constants of the matrix are μ =34.7 GPa and ν =0.3. The



Fig. 3. An infinite plane with a nanocavity and a nanoinhomogeneity under a farfield stress.



Fig. 4. (a) Variation of the hoop stress along the nanocavity boundary when a stiff nanoinhomogeneity is nearby $(\mu_2/\mu=2.0, \sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa). (b) Variation of the hoop stress along the nanocavity boundary when a soft nanoinhomogeneity is nearby $(\mu_2/\mu=0.5, \sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa). (c) Variation of the hoop stress along the interface (on the matrix side) of the matrix and stiff nano-inhomogeneity $(\mu_2/\mu=2.0, \sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa). (d) Variation of the hoop stress along the interface (on the matrix side) of the matrix and soft nanoinhomogeneity $(\mu_2/\mu=0.5, \sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa). (d) Variation of the hoop stress along the interface (on the matrix side) of the matrix and soft nanoinhomogeneity $(\mu_2/\mu=0.5, \sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa).

surface elastic constants and the residual surface tension of the nanocavity are μ_{10} = -6.2178 N/m, λ_{10} =3.48912 N/m, and σ_{10} = 0.72 N/m. Poisson's ratio of the nanoinhomogeneity is taken to be v_2 =0.3, and the shear modulus μ_2 is 17.35 GPa for a soft inhomogeneity and 69.4 GPa for a stiff inhomogeneity. Three cases of parameters are assumed along the interface of the nanoinhomogeneity and matrix. Case I: no surface effects (μ_{20} = λ_{20} = σ_{20} =0); Case II: surface elasticity only (μ_{20} = μ_{10} , λ_{20} = λ_{10} , σ_{20} = σ_{10}). In the numerical calculation, we use 32 and 64 quadratic boundary elements to discretize, respectively, the boundaries of the nanocavity and nanoinhomogeneity. When the matrix is under a remote loading in the *x*- or *y*-direction, our BEM results are in good agreement with those in Ref. [27].

Fig. 4a and b shows the hoop stress variation along the nanocavity boundary when a stiff and soft nanoinhomogeneities are, respectively, nearby. The matrix is under a hydrostatic remote loading $\sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa. The legends "Cases I, II, and III" in Fig. 4a and b represent the results corresponding to the three Cases specified above. Comparing Fig. 4a and b, it is observed that their variation trends are opposite to each other (maximum (minimum) location in Fig. 4b).

Fig. 4c and d depicts the variation of the hoop stress along the interface (on the matrix side) of the matrix and nanoinhomogeneity with both stiff and soft moduli. The matrix is again under a hydrostatic remote loading $\sigma_{xx}^{\infty} = \sigma_{yy}^{\infty} = 100$ MPa. The hoop stress under the hydrostatic loading for the three surface material Cases is nearly identical. Furthermore, a large tensile stress (Fig. 4d) or an oscillatory tensile stress (Fig. 4c) can be observed near the cavity side ($\theta_2 \simeq 180^\circ$). Along the whole interface, the influence of the surface tension and surface elasticity on the stress is negligible. The hoop stress variation on the stiff and soft inhomogeneity side is similar to Fig. 4d, with slightly different magnitude.

4.3. An infinite plane with a square and an equilateral triangle nanoinhomogeneity

A square and an equilateral triangle nanoinhomogeneity made of InAs are embedded in an infinite plane of GaAs subjected to a



Fig.5. An infinite plane with a square and an equilateral triangle inhomogeneity under a far-field stress.



Fig.6. (a) Tangential stress distribution along the interface between the equilateral triangle nanoinhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=1 nm. (b) Tangential stress distribution along the interface between the square nano-inhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=1 nm. (c) Tangential stress distribution along the interface between the equilateral triangle nano-inhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=2 nm. (d) Tangential stress distribution along the interface between the square nanoinhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=2 nm. (d) Tangential stress distribution along the interface between the square nanoinhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=2 nm. (d) Tangential stress distribution along the interface between the square nanoinhomogeneity and matrix under far-field stress $\sigma_{yy}^{\infty} = \sigma_0$, for three interfacial stiffness cases and on both the matrix and inhomogeneity sides, with fixed L=2 nm.

remote loading $\sigma_{yy}^{sy} = \sigma_0$ (Fig. 5). The bulk elastic constants are: $\lambda_1 = 50.66$ GPa, $\mu_1 = 19.0$ GPa for InAs, and $\lambda_M = 64.43$ GPa, $\mu_M = 32.9$ GPa for GaAs. The elastic constants along the interface of the nanoinhomogeneity and matrix are taken to be $\lambda^S = 6.8511$ N/m, $\mu^S = -0.376$ N/m (so that Ks = 6.10 N/m), and $\lambda^S = 3.4939$ N/m, $\mu^S = -5.4251$ N/m (so that Ks = -7.92 N/m) [7]. The side length of the square and triangle is assumed to be the same and is denoted by *L*. The distance between the two nanoinhomogeneities is taken to be L/2 (Fig. 5). Three interfacial stiffness cases are considered, namely, Ks = 0 (corresponding to the traditional no-interface stress case), Ks = 6.10 N/m (positive), and Ks = -7.92 N/m (negative).

We discretize each straight line of the interface between the nanoinhomogeneities and matrix by 6 quadratic elements. The tangential stress along the interface and on both sides of the inhomogeneity and matrix is calculated, and the result is shown in Fig. 6a-d. Fig. 6a shows the tangential stress along the equilateral triangle interface for fixed L=1 nm. In this figure, the labels 01, 12, and 23 on the x-axis denote the triangle side ab, *bc*, and *ca*, respectively. Similarly, Fig. 6b shows the tangential stress distribution along the square interface for fixed L=1 nm, where 01, 12, 23, and 34 on the *x*-axis denote the interfaces *AB*, BC, CD, and DA, respectively. The effect of the interfacial stiffness (Ks=0, 6.10, and Ks=-7.92 N/m) on the stress distribution is clearly demonstrated in these figures. Particularly, it is observed, similar to the previous example, that a negative interfacial stiffness could induce a stress oscillation. For L=2 nm, Figs. 6c and 6d show, respectively, the tangential stress distribution along the triangle and square sides. Along the triangle, the labels 02, 24, and 46 on the x-axis denote the interfaces ab, bc, and ca, respectively, and along the square, the labels 02, 24, 46, and 68 on the x-axis denote the interfaces AB, BC, CD, and DA, respectively. Compared to the small nanoinhomogeneity case in Fig. 6a and b (where L=1 nm), we observe that with the increasing size in inhomogeneities, the interface effect decreases.

5. Conclusions

In this paper, the BEM formulation is extended to include the Gurtin-Murdoch constitutive relation along the interface to study the effect of the surface/interface stresses. Numerical results are compared to existing ones, demonstrating the efficiency and accuracy of the proposed BEM formulation where a nanoinhomogeneity of arbitrary shape can be easily studied. Various nanocavity and nanoinhomogeneity problems are further investigated numerically, including also the interactions between the cavity and inhomogeneity and between a triangle and a square inhomogeneity. These results showed clearly that when the cavity and/or inhomogeneity size is small (say, a couple of nanometers), the surface/interface properties should be incorporated in the study of the elastic behavior of nanoinhomogeneities. Our BEM program can be further extended to the corresponding threedimensional case for analyzing the effect of the surface and/or interfacial stress in nanoinhomogeneities with complicated shapes.

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