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INTERFACIAL STRESSES IN BIMATERIAL COMPOSITES WITH NANOSIZED INTERFACE RELIEF

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Abstract. The paper compares analytical and numerical solutions for two-dimensional solid mechanics problems of elastic bimaterial composites with a nanosized interface relief that arises on a boundary between two bulk layers and on an interface of a nearly circular inclusion. It is supposed that the uniform stress state takes place at infinity. Here, we use Gurtin – Murdoch model in which interphase domains are represented as negligibly thin layers ideally adhering to the bulk phases. Static boundary conditions at the interface are formulated according to the generalized Laplace – Young law. To solve corresponding boundary value we use first-order boundary perturbation method based on Goursat – Kolosov complex potentials. To examine the perturbation results, we use a finite element calculations.

1 INTRODUCTION

At the macrolevel, the effect of surface/interface energy for a stressed solid is ignored as it is small compared to the bulk energy [1]. However, the surface/interface effects become significant for nanoscale materials and structures due to the high surface-to-volume ratio. Stress fields in the vicinity of nanosized structures can appreciably depend on the surface energy and surface stresses, which was first proposed by Gibbs [2]. As a result, the surface/interface stresses are directly related to the size effect, that means the material properties of a specimen depend on its size. To explain the surface phenomena, Gurtin and Murdoch developed the surface elasticity theory [3, 4] which is based on the concept of the surface strain energy and surface stress. The continuum surface/interface stress model assumes that solid consists of bulk and surface phases which are perfectly bonded and have different elastic properties. This theory was confirmed by molecular dynamics simulations [5]. In numerous papers, a finite element modeling was presented to explore the effects of surface/interface stresses in nanoscale structures (see, for example, [6, 7]). In summary, the consideration of these models helps to understand the unusual elastic properties of nanomaterials.

In the work [8], boundary perturbation method (BPM) was used to solve the problem of an elastic infinity plane with a nearly circular inclusion at the macrolevel. The influence of surface stress on an elastic materials containing the nanosized topological defects at external boundary and at internal void boundary was investigated in [9]. Special features of the surface layer behavior in a stressed material particularly is that an initially smooth surface becomes rough under a number of natural phenomena: heat, light, short-wavelength electromagnetic radiation, radioactive emissions, chemicals, mechanical stress, etc. [10]–[14].

Based on the approaches developed in [8, 9, 15], we study the effect of interfacial stresses on stress-strain state of elastic bimaterial with a smooth undulated interface. We consider the 2-D solid mechanics problems of elastic bimaterial composites with a nanometer interface relief that arises between two different bulk layers (the first problem) and between a nearly circular inclusion and a matrix (the second problem). It is supposed that the uniform stress state takes place at infinity. Here, we use Gurtin – Murdoch model [3, 4] in which interphase domains are represented as negligibly thin layers ideally adhering to the bulk phases. Static boundary conditions at the interface are formulated according to the generalized Laplace – Young law [16]. To solve corresponding boundary value we use first-order boundary perturbation method based on Goursat – Kolosov complex potentials. As a result, we come to the hypersingular integral equations in the unknown interfacial stress for any-order approximation of the perturbation procedure. The numerical results are given for a first-order approximation. To examine the perturbation results, we use finite element method (FEM).

2 FORMULATION OF THE PROBLEM

The first problem is following: we consider an elastic isotropic bimaterial with slightly perturbated interface under the uniaxial tension (Fig. 1). It is assumed that the interface profile is defined by the periodic function (1). The interface domain has an elastic properties which differ from the bulk ones. Following Gurtin – Murdoch model of surface elasticity [3, 4], this domain is represented as a negligibly thin layer Γ adhering to the bulk phases B_1 and B_2 without slipping:

$$\Gamma = \{z:\ z = x_1 - i\varepsilon_1 a\cos(bx_1)\}, \quad b = \frac{2\pi}{a}, \quad \varepsilon_1 = \frac{A}{a} \ll 1$$
$$B_1 = \{z:\ x_2 < \varepsilon_1 a\cos(bx_1)\}, \quad B_2 = \{z:\ x_2 > \varepsilon_1 a\cos(bx_1)\}, \tag{1}$$

where a is the wavelength of perturbation, b is the wavenumber and ε_1 is the small parameter.

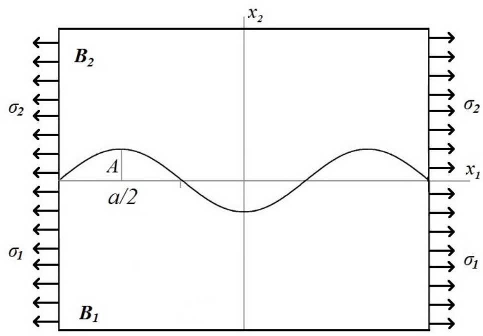


Figure 1: A model of bimaterial with curved interface under uniaxial tension.

The second problem describes an elastic plane with a nearly circular nanoinclusion (Fig. 2). In this case the interface between the matrix and inclusion Γ is defined by the relation:

$$\Gamma = \left\{ z : \ z \equiv \zeta = r \left(1 + \varepsilon_2 \cos 2\theta\right) e^{i\theta} \right\}, \tag{2}$$

where ε_2 is the small parameter which is equal to the maximum deviation of the interface from the circular one of radius r, $\varepsilon_2 > 0$, $\varepsilon_2 \ll 1$.

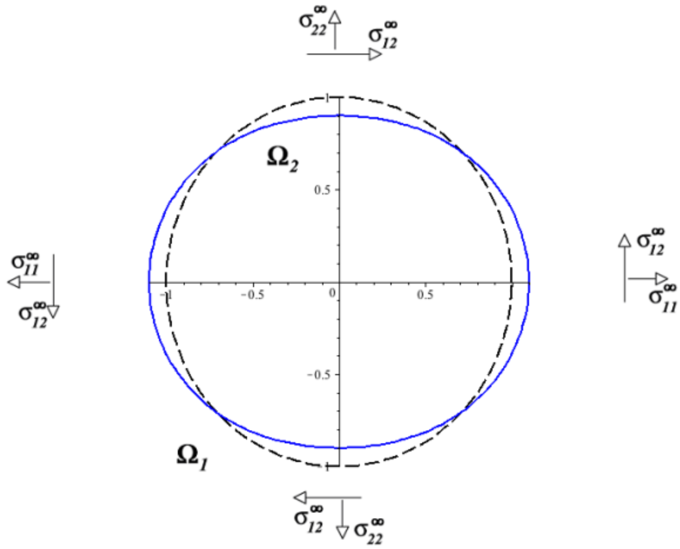


Figure 2: Interface profile of the nanoinclusion described by the cosine function (firm line) for $r = 1$ nm and $\varepsilon_2 = 0,1$.

In equations (1) and (2), $z = x_1 + ix_2$ is the complex variable (i is the imaginary unit). The elastic properties of each domain B_k, Ω_k, $k = 1, 2$, are determined by the Poisson's ratio ν_k and shear modulus μ_k.

We assume that the discontinuity of the displacement on the interface Γ between two domains is absent and the stress jump $\Delta\sigma^k$ ($k = 1, 2$) is determined by the interfacial stress τ according to the generalized Laplace–Young law [9, 15]. The contact conditions can be written in the form

$$\Delta\sigma_n(\zeta) = \sigma_n^+ - \sigma_n^- = \frac{\tau}{R} - i\frac{1}{h}\frac{d\tau}{d\theta} \equiv t^s(\zeta), \quad \Delta u(\zeta) = u^+ - u^- = 0. \tag{3}$$

Stresses σ_{ij} $(i, j = 1, 2)$ and the rotational angle ω of a material particle are specified at infinity as

$$\lim_{z\to\infty} \sigma_{ij} = \sigma_{ij}^\infty, \quad \lim_{z\to\infty} \omega = 0.$$

Here, $\sigma_n = \sigma_{nn} + i\sigma_{nt}$, σ_{nn}, σ_{nt} are the components of stress vector σ_n at the area with the normal $\mathbf{n}$ in the local Cartesian coordinates n, t; $u = u_1 + iu_2$, u_1, u_2 are the displacements along axes of the global Cartesian coordinates x_1, x_2; τ is the interfacial stress. In equation (3), $\sigma_n^\pm = \lim\limits_{z\to\zeta\in\Gamma} \sigma_n(z)$, $u^\pm = \lim\limits_{z\to\zeta\in\Gamma} u(z)$, h is the metric coefficient [17] and R is the curvature radius of the boundary. The superscript "–" corresponds to $z \in B_1$ for the first problem and $z \in \Omega_1$ for the second problem; "+" to $z \in B_2$ and $z \in \Omega_2$, correspondently.

According to [3, 4], constitutive relations of surface and bulk elasticity theory, in the case of the plane strain, are defined as

$$\tau = (\lambda_s + 2\mu_s)\varepsilon_{tt}^s, \quad \sigma_{nt} = 2\mu\varepsilon_{nt}, \tag{4}$$

$$\sigma_{nn} = (\lambda + 2\mu)\varepsilon_{nn} + \lambda\varepsilon_{tt}, \quad \sigma_{tt} = (\lambda + 2\mu)\varepsilon_{tt} + \lambda\varepsilon_{nn}. \tag{5}$$

In equations (4) and (5), σ_{ij} is the stress tensor component,ε_{tt}^s and ε_{ij} are the components of the surface and bulk strain tensors, λ, μ (λ_s, μ_s) are Lame constants of the bulk (surface) material.

From the continuity condition of the displacement, passing from two domains to the interface Γ, we obtain the inseparability condition of the surface and the bulk (see [9, 15, 18]), expressed in terms of hoop strains:

$$\lim_{z\to\zeta} \varepsilon_{tt}^k(z) = \varepsilon_{tt}^s(z), \quad k = 1, 2.$$

3 INTEGRAL EQUATION OF N-ORDER APPROXIMATION

According to [15, 19], the relation of the stresses and the displacements with complex potentials $\Phi_k(z)$ and $\Psi_k(z)$ can be written as

$$G(z,\eta_k) = \eta_k \Phi_k(z) + \overline{\Phi_k(z)} + \left[z\overline{\Phi'_k(z)} + \overline{\Psi_k(z)} \right] \frac{d\bar{z}}{dz},$$

where z is the point anywhere in the domains.

It is important to note that

$$G(z,\eta_k) = \begin{cases} \sigma_n, & \eta_k = 1, \\ -2\mu_k \dfrac{du}{dz}, & \eta_k = -\varkappa_k, \end{cases}$$

where $\varkappa_k = (3-\nu_k)/(1+\nu_k)$ for the plane stress state and $\varkappa_k = 3 - 4\nu_k$ for the plane strain; $dz = |dz|e^{i\alpha}$, $d\bar{z} = \overline{dz}$, α is the angle between the direction $\mathbf{t}$ of the area and the x_1 axis. Functions $\Phi_k(z)$ and $\Psi_k(z)$ are holomorphic in the corresponding domains B_k for the first problem and Ω_k for the second problem.

Following the BPM [8, 9, 15], the complex potentials $\Phi_k(z)$, $\Psi_k(z)$ and the interfacial stress τ are sought in terms of power series in a small parameter ε_k, $k = 1, 2$. The problem is reduced to the solution of two independent Riemann–Hilbert's boundary problems [8]. With the help of Goursat–Kolosov complex potentials, Muskhelishvili's representations [20], the BPM and simplified Gurtin–Murdoch surface elasticity theory, the solution of the first type of the problem leads to the successive solution of hypersingular integral equation in the unknown functions τ_n, $n = 0, 1, \ldots$ [9]

$$\tau'_n(x_1) - \frac{M(\varkappa+1)}{2\pi} \int_{-\infty}^{\infty} \frac{\tau'_n(t)}{(t-x_1)^2} dt = F_n(x_1), \tag{6}$$

and the solution of the second type of the problem leads to the similar equation

$$\left[2a - M(\varkappa-1)\right] \tau_n(\eta) + \frac{M(\varkappa+1)}{2\pi i} \int_{|\xi|=1} \frac{(\xi + \eta^2/\xi)\tau_n(\xi)}{(\xi-\eta)^2} d\xi = G_n(\eta), \quad |\eta| = 1, \tag{7}$$

where $M = (\lambda_s + 2\mu_s)/2\mu$; $\varkappa = (\lambda + 3\mu)/(\lambda + \mu)$; functions F_n, G_n depend on all previous solutions.

4 NUMERICAL RESULTS

The elastic properties are defined by Lame constants $\lambda_1 = 58,17$ GPa, $\mu_1 = 26,13$ GPa for the bulk domains B_1 and Ω_1 and $M = M_1 = 0,117$ nm when $\lambda_s = 6,851$ N/m and $\mu_s = -0,376$ N/m for the interface domain [5, 21]. In this study, we assume elastic properties of the bulk domain B_2 (Ω_2) are related with those for B_1 (Ω_1) as follows: $m = \mu_2/\mu_1 = 1/3$, where m is stiffness ratio. Poisson's ratio $\nu_1 = \nu_2 = 0,34$.

We have verified our numerical results taken from the above first-order approximation by comparing with those of finite element calculations within ANSYS program. The finite element models for two types of considered problems are shown in Fig. 3 and Fig. 4. Following [6], the bulk and the interface layers are considered as different phases with different elastic properties. The model is built of high-order 2-D 6-node triangular elements "plane183" with an intensively-refined mesh near the interface region that allows us to approximate the interface between two phases with high accuracy. The interface region is meshing by 1-D 2-node elements "link180" with unitary cross-section area.

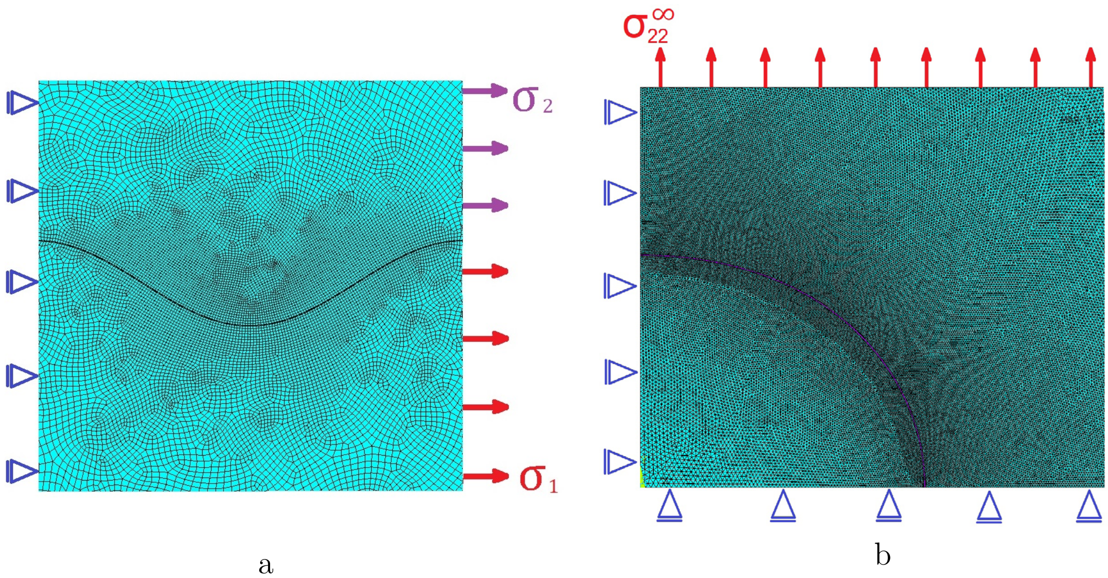
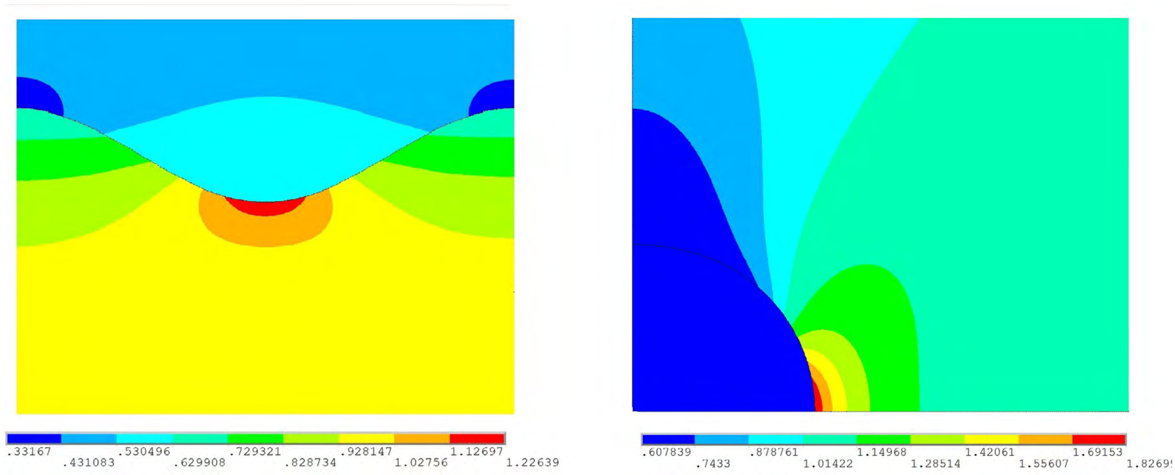


Figure 3: Finite element models of elastic bimaterial composites with the nanometer interface relief that arises between two different bulk phases (one perturbation (a)) and between the nearly circular inclusion and the matrix (quarter of solid (b)) when $\varepsilon_1 = \varepsilon_2 = 0,1$.

Owing to the periodicity of the interface profile for the first problem, it is enough to consider only 5 perturbation periods in the numerical calculation (Fig. 3a). On the symmetry plane ($x = 0$) the displacement u_x is assumed to be zero. The right boundary of the domain B_1 is subjected to a constant load σ_1. Since we assume that the upper half-plane B_2 and lower half-plane B_1 are coherent, the load $\sigma_2 = \sigma_1 m$ is applied on the right boundary of the domain B_2. The interface is considered as domain with elastic properties which differ from those for both bulk phases B_1 and B_2. Using FEM and BPM we studied effect of interfacial stress on the stress-strain state of the bimaterial composite. Fig. 5a reveals the stress concentration factor (SCF) $S_a^1 = \sigma_{tt}^1/\sigma_1$ as a function of perturbation wavelength a for $\varepsilon_1 = 0,1$ and $m = 1/3$. The dotted line is plotted for $M = M_1$ using the first-order approximation of BPM. FEM calculations of SCF S_n^1 for different wavelength



a b

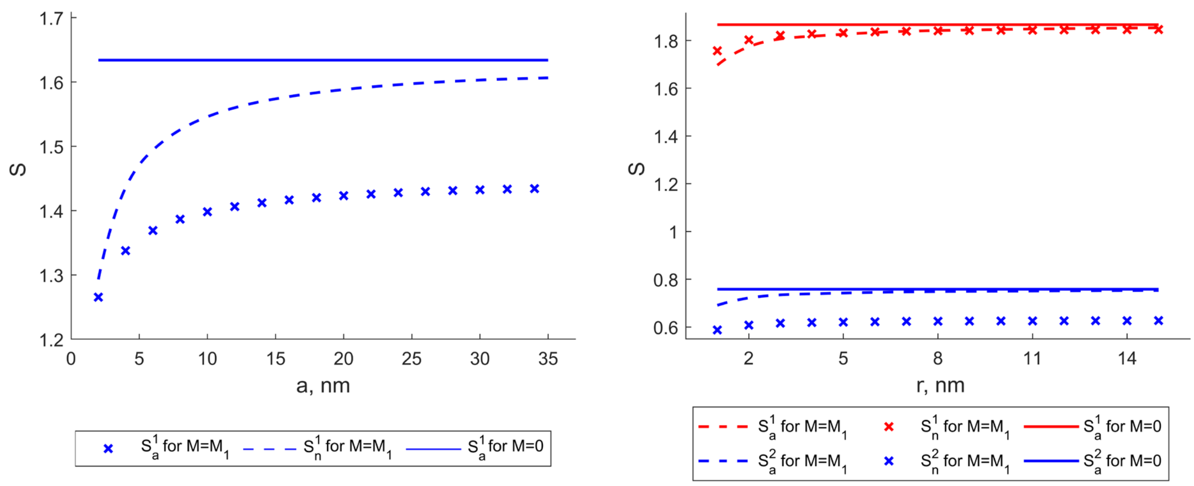
Figure 4: The stress state of the considered problems when $\varepsilon_1 = \varepsilon_2 = 0,1$.

a and $M = M_1$ are marked by crosses. It is shown that both solutions comes to constant values with increase of a. Dashed line correspond to the classical solution ($M = 0$) in the case surface elasticity is neglected.

For the second problem, we investigate the stress field plane containing the nearly circular nanoinclusion with the interface relief described by the function $f(\theta) = \cos 2\theta$ (Fig. 2). Using simplified Gurtin – Murdoch surface elasticity theory and BPM [15], the solution for this problem is reduced to the singular integro-differential equation for any-order approximation (7). For the inclusion described by the cosine function when $\varepsilon_2 = 0,1$ and $r = 2$ nm, in the first-order approximation SCF $S_a^1 = \max \sigma_{tt}^1/\sigma_{22}^\infty$ is equal 1,77 and $S_a^2 = \max \sigma_{tt}^2/\sigma_{22}^\infty$ is equal 0,72, here σ_{tt}^k is hoop stress in the matrix ($k = 1$) and in the inclusion ($k = 2$). Fig. 5b reveals the SCF S_a^k, $k = 1, 2$ ($\theta = 0$) along the boundary of almost circular nanoinclusion for the matrix $k = 1$ (blue lines) and for the inclusion $k = 2$ (red lines) upon the radius r in the case of the uniaxial tension σ_{22}^∞ along axis x_2, i. e., for $\sigma_{11}^\infty = \sigma_{12}^\infty = 0$, $\sigma_{22}^\infty > 0$ when $\varepsilon_2 = 0,1$ and $m = 1/3$. The dotted lines are plotted for $M = M_1$ using the first-order approximation of BPM. FEM calculations of SCF S_n^k, $k = 1, 2$ when $M = M_1$ are marked by crosses. The stress field near the nanoinclusion under the uniaxial tension is shown in Fig. 4b. Dashed lines also correspond to the classical solution when $M = 0$.

5 CONCLUSIONS

We have analyzed the mathematical models of the nanopatterned interphases region of two coherently bonded elastic solids and an elastic body with a nearly circular nanoinclusion. In particular:



a b

Figure 5: Dependence of the SCF S on the wavelength of perturbation a for the first problem (a) and on the inclusion versus radius of the corresponding circular nanoinclusion r for the second problem (b).

- Analytical solutions of considered problems in any-order approximation of BPM is obtained. The effect of interfacial stress on stress-strain state of bimaterial composites near the interface is investigated using first-order approximation. As it was shown, with the increase of the wavelength perturbation a and the radius r of the basic circular inclusion, the maximum hoop stresses at the interface tends to the classical solution when the interfacial stress is not considered. However, with the decrease of the wavelength perturbation a and the radius r, the SCF decreases indefinitely when $M = M_1$. This fact illustrates the size effect as a dependence of the stress state on the size of the interface boundary topological defects.

- To verify the obtained analytical solutions, the considered problems were also solved using FEM. Analytical results for smooth undulated surface when $\varepsilon_1 = \varepsilon_2 = 0,1$ are in a good agreement with FEM calculations. The relative differences between solutions obtained by the describes approaches less than 10% for the first problem and does not exceed 16% for the second problem. Moreover, this results confirmed the previous studies. By increasing the size parameters of the interface boundaries, we came to the solutions obtained in the studies [8, 18], where interface elastic properties was neglected. However, as the small parameter increases, the relative difference between FEM and first-order BPM solutions increase [22, 23]. As a result, it's important to take into account the nonlinear terms of the perturbation solution.

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