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Simulation of ellipsoidal particle-reinforced materials with eigenstrain formulation of 3D BIE

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ABSTRACT

Based on the concepts of eigenstrain and equivalent inclusion of Eshelby for inhomogeneity problems, a computational model and its solution procedure are presented using the proposed three-dimensional (3D) eigenstrain formulation of boundary integral equations (BIE) for simulating ellipsoidal particle-reinforced (and/or void-weakened) inhomogeneous materials. In the model, the eigenstrains characterizing deformation behaviors of each particle embedded in the matrix are determined using an iterative scheme with the aid of the corresponding Eshelby tensors, which can be obtained beforehand either analytically or numerically. With the proposed numerical model, the unknowns of the problem appear only on the boundary of the solution domain, since the interface condition between particles/voids and the matrix is satisfied naturally. The solution scale of the inhomogeneity problem can thus be significantly reduced. Using the algorithm, the stress distribution and the overall elastic properties are identified for ellipsoidal particle-reinforced/void-weakened inhomogeneous materials over a representative volume element (RVE). The effects of a variety of factors on the overall properties of the materials as well as the convergence behavior of the algorithm are studied numerically, showing the validity and efficiency of the proposed algorithm.

1. Introduction

Determination of the elastic behavior of an inclusion embedded in a matrix is of considerable importance in a wide variety of physical and engineering problems. Following the pioneering work of Eshelby [1,2], inclusion and inhomogeneity problems have been a focus of solid mechanics for several decades. Due to Eshelby's work on an equivalent inclusion and eigenstrain solution, numerous investigations both analytical [3–9] and numerical [10–17] have been reported in the literature. In various physical problems, the eigenstrain can represent thermal mismatch, lattice mismatch, phase transformation, microstructural evolution, and intrinsic strains in residual stress problems [18]. Eshelby's solution is of great versatility and has been employed to address a wide range of physical problems in materials science, mechanics, and physics.

The analytical equivalent inclusion models available in the literature can be taken as the basis for predicting stress/strain distribution either within or outside the inhomogeneity and for further study of the mechanical performance of heterogeneous materials. However, the available solutions apply generally to only simple geometries such as single ellipsoidal, cylindrical and spherical inclusions in an infinite domain, because of the complexity of the mathematical expression and difficulty in solving the corresponding governing equations in 3D systems. Therefore, numerical methods including finite element methods (FEM), volume integral methods (VIM) and boundary element methods (BEM) have been used in the analysis of inhomogeneity problems involving various shapes and materials. The FEM may yield results for the entire composite materials, including results within the inhomogeneity [11], but the solution scale would be very large since both matrix and inhomogeneities must to be discretized. The VIM and the BEM seem more suitable than the FEM for the solution of inhomogeneity problems in comparison. In the VIM [12–14], the domains of inhomogeneity are represented by volume integrals, essentially simplifying the construction of the final matrix of the linear algebraic system to which the problem is reduced to some extent after the discretization. However, as the interfaces between matrix and inclusion need to be discretized in the VIM, it is suitable for small scale problems with only a few inhomogeneities. The situation in the application of the BEM to inclusion problems, often coupled with VIM [15,16], is much the same as that of the VIM in which problems of simple arrays of inclusions are solved on a small scale, for a similar reason to that in the VIM, i.e., unknowns appearing in

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the interfaces. For large-scale problems of inhomogeneity with the BEM [17], special techniques of fast multipole expansions [19] must be employed, which leads to complexity of the solution procedure.

To the authors' knowledge, the potential engineering applications of Eshelby's idea of equivalent inclusion and eigenstrain solution have not yet been fully explored in the area of computational treatment of materials with inhomogeneities [20]. With Eshelby's idea as the basis, Ma et al. [21] recently proposed the eigenstrain formulation of the BIE for modeling elliptical particle-reinforced materials in two-dimensional elasticity. In the present work, that computational model is extended to the three-dimensional case by incorporating the corresponding BEM for analyzing the stress/strain behavior of ellipsoidal particle-reinforced/void-weakened materials.

2. Eigenstrain formulations of BIE

In the present model, perfect adhesion between the particle and the matrix, both being isotropic materials, is assumed, so that the displacement continuity and the traction equilibrium still hold true along their interfaces. The solution domain considered is a finite region Ω filled with the matrix and inclusions, bounded by the outer boundary Γ. The domain of the inhomogeneity is denoted by Ω_I with the boundary $\Gamma_I(\Gamma_I = \Omega_I \cap \Omega)$. The displacement and stress fields of the problem can be described by the eigenstrain formulations of the BIE [21,22] as follows:

$$C(p)u_i(p) = \int_\Gamma \tau_j(q)u^*_{ij}(p,q)\,d\Gamma(q) - \int_\Gamma u_j(q)\tau^*_{ij}(p,q)\,d\Gamma(q) + \sum_{I=1}^{N_I}\int_{\Omega_I}\varepsilon^0_{jk}(q)\sigma^*_{ijk}(p,q)\,d\Omega(q) \tag{1}$$

$$C(p)\sigma_{ij}(p) = \int_\Gamma \tau_k(q)u^*_{ijk}(p,q)\,d\Gamma(q) - \int_\Gamma u_k(q)\tau^*_{ijk}(p,q)\,d\Gamma(q) + \sum_{I=1}^{N_I}\int_{\Omega_I}\varepsilon^0_{kl}(q)\sigma^*_{ijkl}(p,q)\,d\Omega(q) + \varepsilon^0_{kl}(p)O^*_{ijkl}(p,q) \tag{2}$$

where

$$O^*_{ijkl}(p,q) = \lim_{\Omega_\varepsilon\to 0}\int_{\Delta\Gamma_\varepsilon} x_l\tau^*_{ijk}(p,q)\,d\Gamma(q) \tag{3}$$

in which Ω_ε (surrounded by the boundary Γ_ε) represents an infinitesimal zone within Ω_I when the source point p approaches the field point q [23] and $x_l = x_l(q) - x_l(p)$. In Eqs. (1) and (2), u^*_{ij}, τ^*_{ij} and σ^*_{ij} stand for the Kelvin's fundamental solutions for displacements, tractions and stresses, respectively. u^*_{ijk}, τ^*_{ijk} and σ^*_{ijk} are correspondingly the derived fundamental solutions [21,22]. N_I is the total number of particles in the domain Ω.

In Eshelby and Mura's terminology [3], an inclusion is a bounded region within a material with the same material properties as the surrounding material but containing a stress-free transformation strain or eigenstrain. In contrast, an inhomogeneity (a particle) existing in a bounded region within a material has different material properties and may (or may not) contain an eigenstrain. Eshelby showed [1,2] that an inhomogeneity under loading can be simulated via an equivalent inclusion containing a fictitious eigenstrain, ε^0_{ij}, expressed by domain integrals in Eqs. (1) and (2), the so-called the eigenstrain formulations. The eigenstrains of particles here are determined using an iterative scheme, which will be described in detail in the following section. Obviously, the eigenstrains in each particle depend on the applied stresses or strains, the geometry of the particle, as well as the material constants of particle and matrix.

Eshelby's original work [1,2] related the constrained strain ε^C_{ij} developed in an inclusion located in an infinite matrix to the eigenstrain (the stress-free strain or the transformation strain) ε^0_{ij} via what is now widely known as the Eshelby tensor S_{ijkl}, that is

$$\varepsilon^C_{ij} = S_{ijkl}\varepsilon^0_{kl} \tag{4}$$

The Eshelby tensor S_{ijkl} is geometry dependent only, and generally takes the form of integrals. For simple geometries, the components of S_{ijkl} can be given explicitly and are available, for example, in the literature [1,4,9] or can be computed numerically [21] by

$$S_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}) + C_{ijmn}\int_{\Gamma_I} x_l\tau^*_{mnk}(p,q)\,d\Gamma = \frac{1}{2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}) + \frac{1}{4\mu}\int_{\Gamma_I} x_l\left\{\tau^*_{ijk}+\tau^*_{jik}-\frac{2\upsilon}{1+\upsilon}\delta_{ij}\tau^*_{mmk}\right\}d\Gamma \tag{5}$$

where C_{ijkl} is the compliance tensor of the matrix, μ the shear modulus. By defining the Young's modulus ratio $\beta = E_I/E_M$, where the subscripts I and M represent the inhomogeneity (particle) and the matrix, respectively, the following relation holds true according to Hooke's law. If a particle is subjected to an applied strain ε_{ij}, it can be replaced by an equivalent inclusion without altering its stress state:

$$(1-\beta_1)\varepsilon^C_{ij} + \beta_2\delta_{ij}\varepsilon^C_{kk} - \varepsilon^0_{ij} - \frac{\upsilon_M}{1-2\upsilon_M}\delta_{ij}\varepsilon^0_{kk} = -(1-\beta_1)\varepsilon_{ij} - \beta_2\delta_{ij}\varepsilon_{kk} \tag{6}$$

where

$$\beta_1 = \frac{1+\upsilon_M}{1+\upsilon_I}\beta, \qquad \beta_2 = \frac{\upsilon_M}{1-\upsilon_M} - \frac{\upsilon_I}{1-2\upsilon_I}\beta \tag{7}$$

and υ is Poisson's ratio. Combining Eqs. (4) and (6), the eigenstrains in each particle can be estimated from the given applied strains.

3. Solution procedures

The present computational model for ellipsoidal particle-reinforced materials is solved numerically by way of the BEM [22]. In order to avoid domain discretization, the domain integrals in Eqs. (1) and (2) need to be transformed into boundary-type integrals before discretization, as [23]

$$\int_{\Omega_I}\sigma^*_{ijk}\,d\Omega = \int_{\Gamma_I} x_k\tau^*_{ij}\,d\Gamma \tag{8}$$

$$\int_{\Omega_I}\sigma^*_{ijkl}\,d\Omega + O^*_{ijkl} = \int_{\Gamma_I} x_l\tau^*_{ijk}\,d\Gamma \tag{9}$$

in which the eigenstrains in each particle are assumed to be constant. It is noted that the applied strains (or the applied stresses) over each particle are disturbed by other particles, especially those near the particle of interest, because the eigenstrain in a particle will induce a self-balanced stress field in both the particle and the matrix. In addition to the applied load, the eigenstrain-induced stresses outside the particle are superimposed on other particles. As a result, the applied strains with regard to the eigenstrains are corrected in an iterative way in the solution procedure. After discretization and incorporated with the boundary conditions, Eq. (1) can be written in matrix form as:

$$\mathbf{A}\mathbf{x} = \mathbf{b} + \mathbf{B}\boldsymbol{\varepsilon} \tag{10}$$

where $\mathbf{A}$ is the system matrix, $\mathbf{B}$ the coefficient matrix for eigenstrains, $\mathbf{b}$ the right vector related to the known quantities applied on the outer boundary, $\mathbf{x}$ the vector unknowns to be solved. $\boldsymbol{\varepsilon}$ is the eigenstrain vector of all the particles to be corrected in the iteration. It should be mentioned that the coefficients in $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{b}$ are all constants, and thus need to be computed only once. At the starting point, the vector $\boldsymbol{\varepsilon}$ is assigned by initial values for the applied