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An advanced 3D boundary element method for characterizations of composite materials

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Abstract

Some recent developments in the modeling of composite materials using the boundary element method (BEM) are presented in this paper. The boundary integral equation for 3D multi-domain elasticity problems is reviewed. Difficulties in dealing with nearly-singular integrals, which arise in the BEM modeling of composite materials with closely packed fillers or of thin films, are discussed. New and improved techniques to deal with the nearly-singular integrals in the 3D elasticity BEM are presented. Numerical examples of layered thin films and composites with randomly distributed particles and fibers are studied. The advantages and limitations of the BEM approach in modeling advanced composites are also discussed. The developed BEM with multi-domain and thin-body capabilities is demonstrated to be a promising tool for simulations and characterization of various composite materials.

Keywords: Boundary element method; Composite materials; Nearly-singular integrals

1. Introduction

Composites have been studied for decades. The anisotropic nature and the configurations in which they are fabricated allow for better design of structures with tailored material properties to meet demanding conditions. Two major categories of composites are available, namely the reinforced composites and the structural composites. Reinforced composites have been ideal material candidates for defense, aerospace and consumer goods industries. Especially, the discontinuously reinforced composites with short fibers or particles are popular since they can be molded into arbitrary shapes by conventional manufacturing techniques [1–3]. Structural composites, traditionally used in aircraft structures, have found recent applications in semiconductor devices and microtransducer systems. Innovations in thin-film deposition techniques result in desirable film qualities and cost-effective volume production of thin films [4–6]. This leads to strong interest in utilizing thin films type of structural composites for the state-of-art applications at the macro and micro-scales. With numerous potential applications, composites are attracting more and more research attentions and their performance are constantly improved to meet the growing challenges.

Characterization of composites thus becomes increasingly important. It is a critical step in understanding new materials before they can be used to build structures. With the increasing complexity in composites being developed, new characterization tools are needed that can analyze, for example, complicated load transfer mechanisms or stress distributions in composite materials. Characterization based on computer simulations has gained increasing interests. Through a representative volume element (RVE), a statistically representative microstructure of a composite, effective material constants can be extracted based on a constitutive model and some well-designed simulations. The advantages of the simulation-based characterization are obvious. For example, it can save the experimental efforts and costs by simply using computer programs to perform repetitive studies.

Numerical methods, primarily the finite element method (FEM) and the boundary element method (BEM), have been used in structural simulation and characterization of

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composite materials for several decades. In the early FEM studies, random microstructures in reinforced composites are simplified into periodic spatial arrangement of inclusions by enforcing periodic boundary conditions. For example, in Refs. [7–9], RVEs with multiple inclusions are studied using the FEM. It is shown in Ref. [8] that FEM simulations are performed on sliced thin portions of random microstructure RVE models due to computational limitations. Refs. [10,11] give some 3D FEM examples of thin films or thin laminated composites. Extremely dense meshes are created near thin material regions involved in these studies, requiring intensive computation. Generally speaking, the domain-based FEM faces many challenges in material simulation. Composite materials often contain arbitrarily thin regions or randomly dispersed inclusions of different size and shapes, yet FEM imposes strict requirement on the element quality such as aspect ratios, skewness and so on in order to ensure the solution accuracy. In order to describe the detailed configuration as well as to have smooth transition at interfaces among different materials, FEM requires extremely fine meshes near these regions, resulting in a large computational model to solve.

It has been shown that the BEM has many distinctive advantages over the FEM for modeling many material related problems [12–19], regarding, e.g. the mesh generation, treatment of thin regions, and accuracy. Among the challenges for the BEM are the issues of singular and nearly-singular integrals, possible domain discretization in nonlinear analysis, and the solution efficiency. However, considerable progresses in these areas have been made for the BEM in recent years. The day when the computational advantages of the BEM over some domain based methods in some applications become too attractive for end users to ignore may not be far away [20].

In this paper, an advanced multi-domain BEM with thin-body capabilities is presented for 3D analyses of various composite materials based on the elasticity theory. Related issues to the BEM in these applications, such as nearly-singular integrals, which are crucial to the successful applications of the BEM to thin shapes, are discussed. Numerical examples using the BEM, including thin films, short-fiber and particle reinforced composites, are presented to demonstrate the effectiveness and potential of the developed 3D multi-domain BEM in modeling and characterization of composite materials.

2. Boundary integral equation formulation and nearly-singular integrals

Composite materials are inhomogeneous and anisotropic in nature, although their constituents, such as the matrix and fibers, can be considered homogeneous, isotropic and linearly elastic. Based on these assumptions and at the constituent level, the following conventional boundary integral equation (BIE) for 3D elastostatic problems can be applied

$$\int_S T_{ij}^{(\beta)}(P,P_0)[u_j^{(\beta)}(P)-u_j^{(\beta)}(P_0)]\mathrm{d}S(P) = \int_S U_{ij}^{(\beta)}(P,P_0)t_j^{(\beta)}(P)\mathrm{d}S(P), \quad \forall P_0 \in S, \tag{1}$$

in which superscript β denotes any single domain of n domains; $u_i^{(\beta)}$ and $t_i^{(\beta)}$ are the displacement and traction fields in that domain, respectively; $U_{ij}^{(\beta)}(P,P_0)$ and $T_{ij}^{(\beta)}(P,P_0)$ the displacement and traction kernels (Kelvin's solution); P the field point (integration point); P_0 the source point (collocation point); and S the domain boundary. BIE (1) is in a weakly-singular form of the conventional BIE and does not involve computations of any singular integrals in the discretization [21,22].

BIE (1) can be applied safely for materials of complex configuration, as long as the nearly-singular integrals, which occurs when the source point P_0 is close to (e.g. the distance to element length ratio is less than 0.1) but not on the surface of integration, can be computed accurately and efficiently. In modeling composite materials, the nearly-singular integrals arise quite often due to the many thin regions present. They must be dealt with accurately to avoid any degradation of simulation results. Earlier efforts for both 3D and 2D BEM have resulted in significant improvements in the accuracy of evaluating nearly-singular integrals. Details of how to handle the nearly-singular integrals in the BEM can be found in Refs. [17,23–29]. Among these research work, the line integral approach [17,27,28] is found to be very efficient. The main idea of this approach is to avoid evaluating the nearly-singular integrals numerically. Instead, the integrals are transformed into line integrals to be evaluated on the contour boundary of a surface element for 3D cases [27,28], or into direct function evaluations for 2D cases [17].

In the line integral approach [27,28], the integral with the traction kernel function in BIE (1) is treated as follows

$$\int_{\Delta S} T_{ij}(P,P_0)u_j(P)\mathrm{d}S(P) = \int_{\Delta S} T_{ij}(P,P_0)[u_j(P)-u_j(P_0')]\mathrm{d}S(P) + u_j(P_0')\int_{\Delta S} T_{ij}(P,P_0)\mathrm{d}S(P), \tag{2}$$

where P_0' (an image point) is the projection of P_0 (source point) on ΔS (a surface element, see Fig. 1).

The essence of the above treatment is that the last term in Eq. (2) can then be transformed into line integrals using the Stokes' theorem and properties of the solid angle integral (see details in Ref. [28]), and that the remaining term in the right-hand side of the equation is at most nearly-weakly-singular. To explain further, consider a polar coordinate transformation $\mathrm{d}S = r'\,\mathrm{d}r'\,\mathrm{d}\theta$, where $r' = |PP_0'|$ and $r = |PP_0|$ (Fig. 1). The integral on the left-hand side of