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A parametric study on probabilistic fracture of functionally graded composites by a concurrent multiscale method

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ABSTRACT

This article reports the results of a parametric study on the fracture behavior of a crack in functionally graded materials. The study involves stochastic descriptions of particle and void numbers; location, size, and orientation characteristics; and constituent elastic properties; a concurrent multiscale model for calculating crack-driving forces; and Monte Carlo simulation for fracture reliability analysis. A level-cut, inhomogeneous, filtered Poisson field describes the statistically inhomogeneous microstructures of graded composites. Numerical results for an edge-cracked, graded specimen show that the particle shape and orientation for the same phase volume fractions have negligible effects on fracture reliability, even for graded materials with a high modular ratio. However, voids and the particle gradation parameter, if they exist or increase, can significantly raise the probability of fracture initiation. Limited crack-propagation simulations in graded composites containing brittle particles reveal that the fracture toughness of the matrix material can significantly influence the likelihood or the extent of crack growth.

1. Introduction

Assessing mechanical reliability of functionally graded materials (FGMs), which possess spatially varying material compositions and microstructures, mandates a fundamental understanding of their deformation and fracture behavior [1,2]. Most existing studies on FGM fracture [3–6] entail calculating crack-driving forces employing smoothly varying material properties that are derived from empirical rules of mixtures, classical bounds, or micromechanical homogenization [7,8]. However, an FGM is a multiphase, heterogeneous material with possibly distinct properties of individual phases. Depending on the crack-tip location and FGM microstructure, the resulting crack-driving forces can be markedly different when a significant mismatch exists in the properties of constituent material phases. Therefore, using homogenized properties in a macroscale analysis may lead to inaccurate or inadequate measures of crack-driving forces and fracture behavior of FGMs. The calculation of crack-driving forces becomes further complicated when accounting for a random microstructure, including spatial and random distributions of sizes, shapes, and orientations of constituent phases [9–12]. Therefore, in general, a stochastic fracture analysis incorporating random microstructural details, particularly in the crack-tip region, is required for high-fidelity reliability analysis [13].

A valuable insight can be gained by investigating how micromechanical parameters, such as the phase volume fraction, location, size, shape, and orientation of particles; porosity; and the fracture toughness properties of constituents, influence the fracture behavior of a particle-matrix FGM. An elaborate computational model, *e.g.*, a microscale model that employs a discrete particle-matrix system in the entire domain of an FGM, can be invoked for such a parametric study. However, a microscale model, although capable of furnishing highly accurate solutions, constitutes a brute-force approach, and is therefore computationally expensive, if not prohibitive. An attractive alternative is multiscale analysis, where effective material properties are employed whenever possible, thereby solving a fracture problem of interest not only accurately, but also economically. For example, a concurrent multiscale model [13], recently developed by the authors, involves stochastic description of an FGM microstructure and constituent material properties, a two-scale algorithm including microscale and macroscale analyses for determining crack-driving forces, and the Monte Carlo simulation for fracture reliability analysis. Numerical results indicate that the concurrent multiscale model is sufficiently accurate, gives fracture probability solutions very close to those generated from the microscale model, and can reduce the computational effort of the latter model by more than a factor of

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two. Therefore, a detailed parametric study can be efficiently conducted using the concurrent multiscale model – the principal focus of this work. In general, the crack-driving forces experienced by an FGM can be very complex in practical scenarios involving a variety of combinations of microstructural parameters and constituent material properties. A clear understanding of the relationship between the microstructure and fracture behavior is vital to the successful application of FGM to the design of mechanical and structural components.

This paper presents the results of a parametric study on fracture behavior of two-dimensional, functionally graded composites. The study involves: (1) stochastic descriptions of particle and void numbers; location, size, and orientation characteristics; and constituent elastic properties; (2) a concurrent multiscale model for determining crack-driving forces under mixed-mode loading; and (3) Monte Carlo simulation for uncertainty propagation and fracture reliability analysis. Section 2 describes a generic fracture problem and a concurrent multiscale model for calculating various fracture response characteristics of interest, defines the random input parameters, and discusses crack-driving forces and fracture reliability. Section 3 describes the Monte Carlo simulation method for calculating statistical moments and probability densities of crack-driving forces, leading to the probability of fracture initiation. A numerical example comprising eight cases of FGM microstructure and three cases of fracture toughness of matrix, and the resultant fracture response, is presented in Section 4. Section 5 provides conclusions from this work and discusses future work.

2. Stochastic fracture mechanics

Consider a three-phase, functionally graded, heterogeneous solid with a rectilinear crack, domain $\mathcal{D} \subset \mathbb{R}^2$, and a schematic illustration of its microstructure, as shown in Fig. 1. The microstructure in general includes three distinct material phases: one phase as particles, another phase as the matrix material, and the remaining phase as voids. The particle, matrix, and void subdomains are represented by $\mathcal{D}_p$, $\mathcal{D}_m$, and $\mathcal{D}_v$, respectively, where $\mathcal{D}_p \cup \mathcal{D}_m \cup \mathcal{D}_v = \mathcal{D}$ and $\mathcal{D}_p \cap \mathcal{D}_m = \mathcal{D}_m \cap \mathcal{D}_v = \mathcal{D}_p \cap \mathcal{D}_v = \emptyset$. A three-phase FGM, henceforth described as a two-phase, porous FGM or simply a porous FGM, can be reduced to a two-phase, non-porous FGM by discarding the void constituent. The particle and matrix represent isotropic and linear-elastic materials, and the elasticity tensors of individual phases, denoted by $\boldsymbol{C}^{(i)}$, are expressed as [14]

$$\boldsymbol{C}^{(i)} := \frac{\nu_i E_i}{(1+\nu_i)(1-2\nu_i)} \mathbf{1} \otimes \mathbf{1} + \frac{E_i}{(1+\nu_i)} \boldsymbol{I}; \quad i = p, m, \tag{1}$$

where the symbol $\otimes$ denotes the tensor product; E_i and ν_i are the elastic modulus and Poisson's ratio, respectively, of phase i; and $\mathbf{1}$ and $\boldsymbol{I}$ are second- and fourth-rank identity tensors, respectively. The superscripts or subscripts $i = p$ and $i = m$ refer to particle and matrix, respectively. At a spatial point $\boldsymbol{x} \in \mathcal{D}$ in the macroscopic length scale, let $\phi_p(\boldsymbol{x})$, $\phi_m(\boldsymbol{x})$, and $\phi_v(\boldsymbol{x})$ denote the volume fractions of particle, matrix, and void, respectively. Each volume fraction is bounded between 0 and 1 and satisfies the constraint: $\phi_p(\boldsymbol{x}) + \phi_m(\boldsymbol{x}) + \phi_v(\boldsymbol{x}) = 1$. The crack faces are traction-free, and there is perfect bonding between the material phases.

Consider a linear-elastic solid with small displacements and strains. The equilibrium equation and boundary conditions for the quasi-static problem are

$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \mathbf{0} \text{ in } \mathcal{D}_p \cup \mathcal{D}_m \text{ or } \mathcal{D} \setminus \mathcal{D}_v \quad \text{and} \tag{2}$$

$$\begin{aligned} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}} \quad & \text{on } \Gamma_t \text{ (natural boundary conditions)} \\ \boldsymbol{u} = \bar{\boldsymbol{u}} \quad & \text{on } \Gamma_u \text{ (essential boundary conditions)}, \end{aligned} \tag{3}$$

respectively, where $\boldsymbol{u} : \mathcal{D} \to \mathbb{R}^2$ is the displacement vector; $\boldsymbol{\sigma} = \boldsymbol{C}(\boldsymbol{x}) : \boldsymbol{\epsilon}$ is the Cauchy stress tensor with $\boldsymbol{C}(\boldsymbol{x})$ and $\boldsymbol{\epsilon} := (1/2)\left(\nabla + \nabla^{\mathrm{T}}\right)\boldsymbol{u}$ denoting the spatially variant elasticity tensor and strain tensor, respectively; $\boldsymbol{n}$ is a unit outward normal to the boundary Γ of the solid; Γ_t and Γ_u are two disjoint portions of the boundary Γ, where the traction vector $\bar{\boldsymbol{t}}$ and displacement $\bar{\boldsymbol{u}}$ are prescribed; $\nabla^{\mathrm{T}} := \{\partial/\partial x_1, \partial/\partial x_2\}$ is the vector of gradient operators; and symbols "." and ":" denote dot product and tensor contraction, respectively.

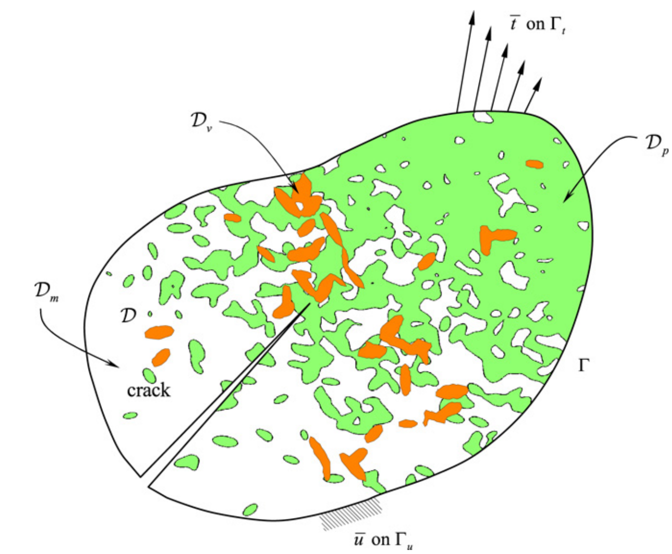

Fig. 1. A crack in a three-phase functionally graded composite. (Note: $\mathcal{D}$ = domain of the entire solid, $\mathcal{D}_p$ = particle subdomain, $\mathcal{D}_m$ = matrix subdomain, $\mathcal{D}_v$ = void subdomain.)

The variational or weak form of Eqs. (2) and (3) is

$$\begin{aligned} &\int_{\mathcal{D}} (\boldsymbol{C}(\boldsymbol{x}) : \boldsymbol{\epsilon}) : \delta\boldsymbol{\epsilon} \mathrm{d}\mathcal{D} - \int_{\mathcal{D}} \boldsymbol{b} \cdot \delta\boldsymbol{u} \mathrm{d}\mathcal{D} - \int_{\Gamma_t} \bar{\boldsymbol{t}} \cdot \delta\boldsymbol{u} \mathrm{d}\Gamma \\ &\quad - \sum_{\boldsymbol{x}_K \in \Gamma_u} \boldsymbol{f}(\boldsymbol{x}_K) \cdot \delta\boldsymbol{u}(\boldsymbol{x}_K) - \sum_{\boldsymbol{x}_K \in \Gamma_u} \delta\boldsymbol{f}(\boldsymbol{x}_K) \cdot [\boldsymbol{u}(\boldsymbol{x}_K) - \bar{\boldsymbol{u}}(\boldsymbol{x}_K)] = 0, \end{aligned} \tag{4}$$

where $\boldsymbol{f}^{\mathrm{T}}(\boldsymbol{x}_K)$ is the vector of reaction forces at a constrained node K on Γ_u, and δ denotes the variation operator. The discretization of the weak form, Eq. (4), depends on how the elasticity tensor $\boldsymbol{C}(\boldsymbol{x})$ is defined, *i.e.*, how the elastic properties of constituent material phases and their gradation characteristics are described. In the following section, a concurrent multiscale model is described to approximate $\boldsymbol{C}(\boldsymbol{x})$. Nonetheless, a numerical method, *e.g.*, the finite-element method (FEM), is generally required to solve the discretized weak form, providing various response fields of interest.

2.1. Concurrent multiscale model

The FGM microstructure in Fig. 1 contains discontinuities in material properties at the interfaces between the matrix and particles. There exist two approaches with respect to defining the material property for fracture analysis of an FGM cracked structure. One approach involves stress analysis using effective material properties, often smooth and continuous, in the entire domain of the solid. This approach is referred to as macroscale analysis. The other approach, referred to as microscale analysis, entails stress analysis that is solely based on the exact but discrete material property information derived from the knowledge of explicit particle locations and their geometry. The concurrent multiscale model employed in this work includes both continuous and discrete material representations and requires a combined micromechanical and macromechanical stress analysis.