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Coupled continuum and discrete analysis of random heterogeneous materials: Elasticity and fracture

Leon S. Dimas, Tristan Giesa, Markus J. Buehler *

Laboratory for Atomistic and Molecular Mechanics (LAMM), Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA, USA

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ABSTRACT

Recent work has suggested that the heterogeneous distribution of mechanical properties in natural and synthetic materials induces a toughening mechanism that leads to a more robust structural response in the presence of cracks, defects or other types of flaws. Motivated by this, we model an elastic solid with a Young's modulus distribution described by a Gaussian process. We study the pristine system using both a continuum and a discrete model to establish a link between the microscale and the macroscale in the presence of disorder. Furthermore, we analyze a flawed discrete particle system and investigate the influence of heterogeneity on the fracture mechanical properties of the solid. We vary the variability and correlation length of the Gaussian process, thereby gaining fundamental insights into the effect of heterogeneity and the essential length scales of heterogeneity critical to enhanced fracture properties. As previously shown for composites with complex hierarchical architectures, we find that materials with disordered elastic fields toughen by a 'distribution-of-weakness' mechanism inducing crack arrest and stress delocalization. In our systems, the toughness modulus can increase by up to 30% due to an increase in variability in the elastic field. Our work presents a foundation for stochastic modeling in a particle-based micromechanical environment that can find broad applications within natural and synthetic materials.

1. Introduction

Materials typically exhibit heterogeneous characteristics at different length scales and in various forms, including the ordered heterogeneous distribution of stiffness in mineralized composites and the disordered distribution of impurities and grain boundaries in solids and the disordered porous networks of clays and soils (Gupta et al., 2006; Harter and Yeh, 1998; Kumar et al., 2009, 2011; Tai et al., 2007; Younis et al., 2012; Zhang et al., 2012). The fracture mechanics of composite material systems exhibiting ordered distributions of heterogeneous properties, both synthetic and natural, are well studied from an experimental, computational, and theoretical standpoint (Aizenberg et al., 2005; Barthelat et al., 2007; Dimas and Buehler, 2012; Fratzl et al., 2007; Gao et al., 2003; Kumar et al., 2011; Okumura and de Gennes, 2001; Waddoups et al., 1971; Whitney and Nuismer, 1974; Zhang et al., 2012). These studies underline the significance of contrast in material properties between the material's constituents as well as their respective placement to within the material achieve enhanced mechanical properties.

* Corresponding author.
E-mail address: mbuehler@MIT.EDU (M.J. Buehler).

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Apart from composite materials, i.e. materials with ordered heterogeneous properties, there has been considerable research of fracture in material systems that exhibit disordered heterogeneous mechanical properties (Bolander and Saito, 1998; Curtin, 1997; Curtin and Scher, 1990; Kumar et al., 2011; Sahimi and Arbabi, 1993). However, only Tai et al. (2007) have used a continuum model to analyze fracture in materials with disordered heterogeneity. Other continuum level efforts have been focused on the elastic response of solids. Many of these studies followed from the seminal work of Ghanem and Spanos (1990), Spanos and Ghanem (1989). Their research presented a spectral method for propagating disorder and uncertainty through differential equations in terms of Karhunen–Loeve (KL) expansions and polynomial chaos (PC) expansions. Following these contributions, other studies have devised similar frameworks resulting in a comprehensive treatment of uncertainty and disorder in natural systems (Le Maitre et al., 2001; Matthies et al., 1997; Xiu et al., 2002).

Fracture is a multi-scale phenomenon that involves breaking bonds at the nanoscale and structural failure at the macroscale (Anderson, 2005; Buehler, 2008; Buehler and Xu, 2010; Griffith, 1921; Gross and Seelig, 2011). An important task in the analysis of the mechanics of solids is thus to develop models capable of predicting material behavior at multiple length-scales. Various research efforts have focused on this task, resulting in several multi-scale analysis methods (Gao and Klein, 1998; Shenoy et al., 1999; Shilkrot et al., 2004). Here, we propose a new method advancing towards a unified framework in which disordered distributions of heterogeneous mechanical properties can be modeled in both continuum and discrete systems. Heterogeneity can arise in material systems in many different forms, and we therefore aim to study its implications as generally as possible. In order to explicitly study disordered systems it is necessary to choose a particular model of disorder. To study disorder in a general manner, this model is ideally as neutral as possible. The concept of neutrality is explained in detail in the materials and methods section. Although we confine the study to one specific description of heterogeneity, the framework presented here is valid for an array of heterogeneity descriptions.

We analyze the case of a two-dimensional solid with a heterogeneous distribution of Young′s modulus modeled as a Gaussian process (Karhunen, 1946; Loeve, 1955; Xiu and Karniadakis, 2002). We then validate the persistence of the Cauchy–Born rule in the presence of disorder. Finally, we apply this model to study the fracture mechanical properties of discrete stochastic systems. Considering the linear relation between strain energy density and Young′s modulus, the model would suggest the fracture toughness modulus of the specimen ensemble to be symmetrically distributed around the mean of the homogeneous system. However, the specimen ensemble features an asymmetric toughness modulus distribution with a positive skewness and a mean value significantly higher than that for homogeneous systems. This work elucidates toughening mechanisms induced by heterogeneous stiffness distributions and the specific parameters of the random stiffness fields.

2. Materials and methods

2.1. Stiffness field

We describe the disordered elasticity field E of the solid as a two-dimensional Gaussian random field with mean $\mu_E = 100$, this arbitrary value is chosen for mathematical convenience, and write

$$E(x_1, x_2) = E_0 + \mathrm{GP}(\boldsymbol{\mu}, \boldsymbol{\Sigma}). \tag{1}$$

In Eq. (1), $\boldsymbol{\mu}$ is the mean of the Gaussian random field. For our model system, all parameters are unitless. Accordingly, we prescribe $\boldsymbol{\mu} = 0$, thus implying $E_0 = 100$.

By choosing a Gaussian process as opposed to a log-normal process, realizations of negative stiffness are possible with large enough variabilities of the Gaussian process (GP). Although we do not wish to study negative stiffness materials here, it is sensible to utilize a Gaussian process due to its inherent symmetry. By confining the variability of the process we limit the number of realizations of negative stiffness to a negligible amount.

This study aims to isolate the effect of heterogeneity on the elastic and fracture response of materials. With a log-normal process, the stiffness distribution would be skewed towards above mean stiffness. This could induce bias on the mechanical properties of the modeled systems when compared to a purely symmetrical system. The symmetry of the Gaussian process enforces a neutral description of heterogeneity. This means that the disorder affects only a controlled amount of system properties and that each realization of a mechanical property above the mean is accompanied by a corresponding realization below the mean. Therefore, the system properties are designed to be symmetric.

We use a simple, convenient form of the covariance matrix $\boldsymbol{\Sigma}$. We choose a stationary exponential kernel write it as

$$\boldsymbol{\Sigma}(\boldsymbol{x}, \boldsymbol{x}') = \sigma_E^2 \exp\left(-\frac{|x_1 - x'_1|}{\alpha \times L} - \frac{|x_2 - x'_2|}{\alpha \times L}\right). \tag{2}$$

In Eq. (2), σ_E^2 is the variability of the Gaussian process and $\alpha \times L$ is the correlation length, with α denoting the correlation length parameter and L denoting the length of the system in the x_1- and x_2-direction respectively. This correlation kernel is common for studies developing new models and methods (Le Maitre et al., 2001; Spanos and Ghanem, 1989). To the best of the authors' knowledge, this paper represents the first study in which heterogeneity is modeled explicitly as a Gaussian process for discrete material systems.