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Modeling fracture of random media via stochastic molecular mechanics LEON DIMAS, TRISTAN GIESA, MARKUS BUEHLER, Massachusetts Institute of Technology — Inspired by recent experimental results suggesting that the heterogeneous distribution of the elastic modulus in bone tissue leads to increased toughness, we determine the toughness modulus of a flawed discrete particle system with stochastic elastic properties. We consider an elastic solid in plane strain conditions in uniaxial tension with a Young's modulus distribution modeled as a 2-d Gaussian process with covariance modeled as an exponential kernel. We solve the problem from a continuum perspective, both employing spectral methods with stochastic finite elements and Monte Carlo methods with conventional finite elements. We also analyze an equivalent discrete particle system, modeled as a spring bead network of FCC-lattices. Our results validate the persistence of the Cauchy Born rule in a stochastic system. We then analyze a flawed discrete particle system to assess the effect of heterogeneity on fracture properties. By studying the fracture mechanics of this system with a range of variance and correlation length parameters in the exponential kernel we gain fundamental insights in to the essential length scales of heterogeneity critical to enhanced fracture properties. This validated stochastic molecular mechanics framework further supports the inverse computation of local elastic properties, not accessible with continuum mechanics, to tailor global mechanical properties such as the fracture toughness. Specifically, Markov Chain Monte Carlo can be used to infer the elastic and geometric parameters. Our work sets the foundation for stochastic modeling in a micromechanical environment and unveils mechanisms by which mechanical behavior can be tailored due to increasingly heterogeneous mechanical properties.

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