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An upscaled law for fractured Carbon nanotubes

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Abstract

Notwithstanding its recent focus on microstructure-driven non-classical aspects, a breakthrough model in continuum mechanics that can evolve the macroscopic deformation of a solid body undergoing fracture whilst systematically incorporating the microstructural information remains elusive. In addressing this issue, we presently obtain, based on the molecular level information, a derivative-free balance law pertaining to a higher scale of interest and useful in a continuum or discrete setting. Derived using a probabilistic projection technique, the law exploits certain microstructural information in a weakly unique manner. The projection generalizes the notion of directional derivative and, depending on the application, may be interpreted as a discrete Cauchy–Born map with the structure of the classical deformation gradient emerging in the infinitesimal limit. As an illustration, we use the Tersoff–Brenner potential and obtain a discrete macroscopic model for studying the deformation of a single-walled carbon nanotube (SWCNT). The macroscopic (or continuum) model shows the effect of chirality – a molecular phenomenon – in its deformation profile. We also demonstrate the deformation of a fractured SWCNT, which is a first-of-its-kind simulation, and predict crack branching phenomena in agreement with molecular dynamics simulations. As another example, we have included simulation results for fractured SWCNT bundle with a view to establishing our claim regarding the efficacy of the proposed method.

Keywords: Carbon nanotube, crack growth, Upscaling, stochastic projection

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