Continuum Shape Sensitivity Analysis and What-if Study for Two-dimensional Multi-scale Crack Propagation Problems Using the Bridging Scale Method

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Abstract

Crack propagation in structural components is an outstanding issue in the field of mechanical design. Theoretical fracture models are generally empirical in nature, and are therefore limited in revealing the crack propagation mechanism at microscopic level. Due to the rapid advances in computation power, molecular dynamics has become a prominent tool for studying and understanding the fundamental mechanism in crack propagation. In this paper, a shape sensitivity analysis approach for two-dimensional multi-scale crack propagation problems is presented. The sensitivity analysis is based on a continuum formulation of the bridging scale decomposition, which is a recently developed multi-scale method that provides an efficient way of coupling simulations of different length and time scales. With the bridging scale method, the computation of atomistic responses becomes affordable since molecular dynamics simulations are performed only within localized regions where atomistic scale physical phenomena are of interest. As the extension of a previous study, the sensitivity formulation in this paper allows the structure to be modeled with irregular-shaped finite elements. Moreover, as a first attempt, we investigate how macroscopic shape change affects crack propagation at microscopic level. In molecular dynamics simulations, the crack length is usually measured with a prescribed criterion that cannot be formulated as a continuous function of shape design variables. Therefore, we propose a hybrid method that combines analytical sensitivity analysis with finite difference approach. In this hybrid method, the sensitivity of atomistic responses, including the displacements, velocities and accelerations of all atoms, is first calculated analytically using the direct differentiation method of the shape DSA; the results are then used to predict the atomistic responses, and thus crack propagation speed in a perturbed structure; the sensitivity of crack growth rate is approximated based on the difference between the perturbed crack propagation rate and that of the current design. Furthermore, we evaluate and compare several performance measures that quantify crack propagation speed based on crack tip locations for sensitivity analysis. A two-dimensional beam example is presented to demonstrate the accuracy of the proposed approach. It is found that the sensitivity accuracy for crack propagation speed is closely related to the choice of the performance measure. In addition, through a what-if study, it is demonstrated that with an adequate performance measure, the impact of macroscopic shape change on microscopic crack propagation speed can be accurately predicted. Although the nearest neighbor Lennard-Jones 6-12 potential used in our examples is too general to represent the potential of a specific material, it is capable of capturing key phenomena that are related to microscopic fatigue fracture. The L-J potential can be replaced by other potentials that represent specific materials while applying the proposed method for a specific application. The sensitivity analysis results can be applied to support fatigue-life-based shape optimization for arbitrary shaped two dimensional structures.

***Keywords**: bridging scale method, cyclic loading, shape sensitivity analysis.*

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