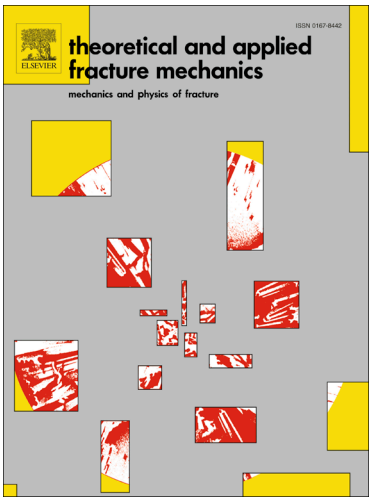

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A three dimensional adaptive multiscale method for crack growth in Silicon

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Abstract

A three dimensional concurrently coupled adaptive multiscale method is introduced here to simulate complex crack growth patterns in Silicon, by combining several numerical techniques across the length scales. The coarse scale material is modeled using the virtual atom cluster model. The strong kinematic discontinuities in the bulk are modeled based on a three dimensional version of the phantom node method. A molecular statics model placed around the crack tip, is concurrently coupled with the phantom-based discontinuous formulation, where the coupling between the fine and coarse scales is realized through the use of ghost atoms. The ghost atoms positions are interpolated based on the coarse scale solution. The boundary conditions to the fine scale model, at the coupling region, are achieved by enforcing the interpolated displacements of ghost atoms. In order to optimize the computation costs, adaptivity schemes for adjustment of the fine scale region as the crack propagates and coarse graining of the region behind the crack tip are proposed. The crack tip location is detected based on an energy criterion. All the molecular simulations in the pure atomistic as well as the multiscale model are carried out using the LAMMPS software. The LAMMPS is triggered through the `system` command in MATLAB. The developed framework is assessed through several numerical examples, focused on the study of crack growth in Silicon. Therefore, the diamond cubic lattice structure of Silicon is used at the fine scale, where the atom-atom interactions are modeled based on the Tersoff potential function. According to the numerical examples presented in this study, savings in computational time using the present multiscale method are observed to be upto 87%, as compared to the pure atomistic model. Furthermore, the studied applications show the robustness and versatility of the proposed methodology.

Keywords: Multiscale analysis; Three dimensional fracture; Atomistic simulations; Silicon; Adaptivity.

1. Introduction

Investigating the material behaviour at the smallest scale provides valuable information regarding the physical behavior of materials, especially in detecting material failures [1]. However, there are other mechanical aspects of vital importance in heterogeneous materials, such as the comprehensive understanding of the influence of hierarchical organizations and multiphase interfaces across length scales on macroscale properties, and the prospective presence of defects, to name a few of them. The exploitation of this information will provide an excellent potential for developing a materials-by-design approach for novel engineering materials and cyberphysical material systems [2]. In this context, although the discrete MD simulations promise to reveal the fundamental mechanics of material failure, the atom dimensions of the order of angstroms (Å) made them still prohibitively expensive to be employed in regular industrial applications [3, 4].

Due to the present computational limitations, the advent of multi-scale modeling procedures opened a new scenario. Among the different multi-scale methods, a possible alternative to reduce the numerical demands envisages the coupling the discrete scale with the continuum scale using continuum-atomistic approaches. In such scenarios, a self-consistent continuum model is defined over the entire domain under analysis, while the defects are explicitly modeled at the sub-scales. Adopting this computational approach, several numerical models dealing with multiple temporal and spatial length scales have been developed in the last two decades [5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. Most of the coupling methods and simulations have been focussed on simulation of materials without cracks. However, the transfer of information across the length scales for problems involving material failure and finite temperatures still remains a challenging task. A thermodynamically consistent

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