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Concurrently coupled solid shell based adaptive multiscale method for fracture

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Abstract

A solid shell-based adaptive atomistic-continuum numerical method is herein proposed to simulate complex crack growth patterns in thin-walled structures. A hybrid solid shell formulation relying on the combined use of the enhanced assumed strain (EAS) and the assumed natural strain (ANS) methods has been considered to efficiently model the material in thin structures at continuum level. The phantom node method (PNM) is employed to model the discontinuities in the bulk. The discontinuous solid shell element is concurrently coupled with a molecular statics model placed around the crack tip. The coupling between the coarse scale and fine scale is realized through the use of ghost atoms, whose positions are interpolated from the coarse scale solution and enforced as boundary conditions to the fine scale model. In the proposed numerical scheme, the fine scale region is adaptively enlarged as the crack propagates and the region behind the crack tip is adaptively coarsened to optimize the computation costs. An energy criterion is used to detect the crack tip location. All the atomistic simulations are carried out using the LAMMPS software. A computational framework has been developed in MATLAB to trigger the LAMMPS through `system` command. This allows a two way interaction between the coarse and fine scales in MATLAB platform, where the boundary conditions to the fine region are extracted from the coarse scale and the crack tip location from the atomistic model is transferred back to the continuum scale. The developed framework has been applied to study crack growth in the energy minimization problems. Inspired by the influence of fracture on current-voltage characteristics of thin Silicon based photovoltaic cells, the cubic diamond lattice structure of Silicon is used to model the material in the fine scale region, whilst the Tersoff potential function is employed to model the atom-atom interactions. The versatility and robustness of the proposed methodology is demonstrate by means of several fracture applications.

Keywords: Multiscale analysis; Solid shell; Phantom node method for fracture; Atomistic simulations; Adaptivity; Silicon solar cell.

1. Introduction

In engineering applications, the global response of the system is often governed by the material behaviour at small length scales. For example, the macroscopic properties of a material such as toughness, strength and ductility are strongly influenced by small scale defects like cracks and dislocations, which are initiated and evolve at the micro and nano scales. Hence, in the ambitious aim to derive the overall full-scale global mechanical response using a bottom-up approach, the sub-scale behaviour has to be accurately computed. Although molecular dynamics (MD) simulations promise to reveal the fundamental mechanics of material failure by modeling the atom interactions, they are still prohibitively expensive to be employed in industrial applications [1, 2]. Therefore, a plausible alternative to reduce the computational demand is to couple the continuum scale with the discrete scale using a multiscale approach.

In this concern, the Quasi-Continuum Method (QCM) developed in [3] constitutes a new frontier for the formulation of novel multiscale methods coupling atomistic and continuum domains. In the QCM, the continuum degrees of freedom need to be located at the positions of the atoms at the interface, requiring a very fine grading of the continuum mesh around the defects. In two scale coupling, concurrent multiscale methods are mainly distinguished based on the coupling domain as the 'Interface' and 'Handshake' coupling. The coupling is achieved across the boundary in the former case, whereas the regions are coupled over a finite overlapping domain in the latter approach. Classical examples of the 'Interface' and 'Handshake' coupling are the bridging scale method (BSM) and the bridging domain method (BDM), respectively. In particular, the BSM is based on

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