An adaptive eXtended Bridging Scale Method for crack propagation

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ABSTRACT

An adaptive eXtended Bridging Scale Method (XBSM) method is developed to analyse the coupled continuum-atomistic model for crack propogation studies using the minimum energy criteria. Cracks in the atomistic domain are modelled by removing the bonds between the atoms and phantom node method is used to model the crack in the continuum domain. Furthermore, the Virtual Atom Cluster (VAC) model is used to model the coarse scale domain. The ghost atom positions are interpolated from the continuum solution and enforced as the boundary conditions for the fine scale solution. The fine scale region is adaptively enlarged as the crack propagates and the model behind the crack tip is coarsened to reduce the size of the fine scale region. An energy criterion is used to detect the crack tip location. The method is implemented for two dimensional models with triangular lattice corresponding to the [111] plane of an FCC crystal. The results show good agreement between molecular and continuum models.

In this paper we present a coupled, multiscale, continuum-atomistics model based on the extended finite element method (XFEM) and Bridging Scale Method (BSM). We name this method eXtended Bridging Scale Method (XBSM). The atomistic subdomain is denoted the ”fine scale region” and to the continuum subdomain the ”coarse scale region”. The coarse region is present everywhere in the domain. A crack in the fine scale region is created by removing the bonds between the atoms and updating the neighbor list accordingly. Nodal displacements in the coarse region are estimated using the VAC model [1]. The VAC model is based on the repetitiveness of a set of atoms in the entire crystal. The advantage is that a cluster of atoms can represent the energy density as defined at any point within this structure. As a result all the calculations can be performed with regard to the cluster, which otherwise would need to be carried out at each and every atom. Hence the computational efficiency

of the model improves drastically. The link between the VAC model and the original atomistic model can be established by adopting the same inter atomic potential as in the full scale MD simulations. The phantom node method [2] is used to simulate the crack in the coarse scale region. In the Phantom node method the cracked element is modeled as two elements. Ghost atoms are located in the coarse region that is within the cutoff radius of the atoms in the fine region. Ghost atom positions are interpolated from the coarse scale solution and enforced as the boundary conditions for the fine scale solution. The crack originates from the coarse region with the crack tip in the fine region. The fine scale region is adaptively enlarged as the crack propagates and the model behind the crack tip is coarsened to reduce the size of the fine scale model [3] and [4]. An energy criterion is used to detect the crack tip location. The method is implemented for two dimensional models.

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