A multiscale model for amorphous materials

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A B S T R A C T

In this work, we proposed a Cauchy-Born rule (CBR) based multiscale model to study mechanical properties of amorphous materials. In this work, we combine a coarse-grained Parrinello-Rahman (CG-PR) method and the Multiscale Cohesive Zone Method (MCZM) method to model the Lennard-Jones (L-J) binary glass and amorphous silicon (a-Si) solid. The proposed CG-PR method applies the CBR to a representative volume element of an amorphous material with representative microstructure pattern, whose side dimension is about twice of the cutoff distance of interatomic interaction. Numerical simulations were carried out, and it is found that the CG-PR method can reproduce stress-strain relations extrapolated from large scale MD simulations for both L-J binary glass as well as amorphous silicon (a-Si).

The CG-PR method is then combined with MCZM method to simulate failure process of amorphous materials. We found that (1) the CG-PR method can capture the history-dependent inelastic stress-strain relation in amorphous materials, and (2) the CG-PR enhanced MCZM method can simulate both brittle and ductile fracture in both a-Si solid and L-J binary glass. Moreover, the multiscale methodology developed here may be extended to study mechanical properties of a variety of other non-crystalline materials.

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1. Introduction

The Cauchy-Born rule (CBR) is basically a kinematic assumption on atoms motions in crystalline materials. Utilizing the CBR assumption, one can develop multiscale methods to construct macroscale constitutive models for crystalline materials, which are informed by atomic or molecular information at microscale. Historically, Cauchy assumed that the macroscale deformation motion and the atomistic movement in multiplying scale factor. This concept was further extended by Born who introduced macroscopic deformation gradient as a linear transformation of position vectors in the reference configuration to describe atom arrangements [1]. By assuming that both kinematic motions in macroscale and microscale are affine deformation, many multiscale models have been developed to establish constitutive models for various crystalline solids by utilizing with interatomic interaction potentials, e.g. [2–4] among others.

In specific, because that the Cauchy-Born rule assumes uniform deformation in crystalline solids, we can estimate atom positions r in deformed configuration simply as r = F R, where F is the deformation gradient, and R is referential coordinate of atom. For example, the local form of the quasi-continuum (QC) method [2,3] uses the interpolation field among the representative atoms to describe a continuous atomistic displacement field, which provides an estimate for each atom’s displacement in the domain. Multiscale Cohesive Zone Model (MCZM) [4,6] applies the same technique to a MD unit cell consisting of multiple atoms, which is assigned to each quadrature point inside an (finite) element. Since the unit cell is embedded in each quadrature point of a finite element, we can use it to evaluate both constitutive relation as well as the cohesive law at that material point. This procedure provides great advantage to evaluate stress-strain relation for crystalline solids, especially for single crystals. This is because that in each element one only needs to calculate stress at the locations of a few quadrature points. As a result of such simplification, computational cost is greatly reduced to simulate material behaviors at macro-scale based on microscale information. For example, as the Bravais lattice, both face-centered (FCC) and body-centered cubic (BCC) crystals have only one atom in their Wigner-Seitz cells. When evaluating stress at one quadrature point, one only needs to calculate atomistic interaction around that atom, which are only involved with a few dozen neighboring atoms. For non-Bravais lattices, for example the cubic diamond crystal, its lattice structure may be considered as a pair of interpenetrating FCC lattices, thus it is also

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