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A multiscale model for amorphous materials

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ABSTRACT

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 Model (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 CG-RP method can reproduce the 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.

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 $\mathbf{r}$ in deformed configuration simply as $\mathbf{r}_i = \mathbf{F} \cdot \mathbf{R}_i$, where $\mathbf{F}$ is the deformation gradient, and $\mathbf{R}_i$ is referential coordinate of atom. For example, the local form of the quasi-continuum (QC) method [2,5] 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 macroscale 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-Bravie 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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possible to apply CBR by adding additional degree of freedom that represents the distance between two atoms inside its Wigner-Seitz cell [6,7].

Based on this technique, a number of multiscale methods have been developed for crystalline materials whose lattices resemble the diamond crystal lattice such as silicon or other semiconductor crystals e.g. [2,8,9]. On the other hand, the Cauchy Born rule has been extended to include nonlinear deformation by considering the contribution of higher order deformation gradients. For examples, Sunyk and Steinmann have applied the higher order Cauchy-Born rule in crystalline solids with inhomogeneous deformation by considering the second order deformation [10]. CBR has also been applied to membrane sheets of graphenes, thin plates of mutilayer graphenes, and nanowires by introducing the so-called exponential CBR that takes into account the curvature effect in deformation mapping [11,12]. In order to distinguish bulk crystal and crystal surface region, Park et al. proposed the concept of the surface CBR [13], and they also applied the method to study surface effect on silicon [14]. Khoei et al. further extended the idea to take in account of corner and edge effects on microscale silicon [15]. Li et al. have applied up to fourth order CBR to describe different types of crystal defects to study dislocation dynamics [16].

Contrary to single crystal materials, studies of multiscale modeling for amorphous materials are relatively limited, despite of the fact that there exist a large variety of amorphous materials, such as glasses, ceramics, amorphous semiconductors and various polymer materials, in engineering applications. This is largely due to the complexity and difficulty in amorphous material modeling [17]. Most of amorphous material modelings are restricted at the mesoscale level by using the homogenization methodology in micromechanics [18], for example, using the approach of Eshelby's equivalent inclusion method [19], which assumes a homogeneous material with equivalent eigenstrains corresponding to heterogeneous material. For instance, Liu and Sun employed the method to estimate effective elastic stiffness and yield strength of amorphous nanocomposites [20].

However, recently, Albaret et al. attempted to connect micromechanics approach with molecular dynamics approach by combining the Eshelby inclusion method with molecular dynamics (MD) simulations to study amorphous silicon material [21]. Valavala et al. also tried to predict hyperelastic continuum constitutive relation for Polyimide and Polycarbonate based on MD simulations [22]. Other efforts have been made for multiscale modeling of amorphous polymers. The Pseudo-Amorphous Cell (PAC) method employs representative volume elements (RVE) to model amorphous materials, in which atom displacements are related to the cell deformation without assuming continuous displacement field by using so-called transformation matrix operator for small deformation regions [23–25]. The RVE approach in micromechanics is also applied to amorphous polymetric material by coupling molecular dynamics calculations with the finite element calculations [26]. Almost of all these studies adopt micromechanics homogenization scheme to build a hierarchical modeling, but no CBR technique has ever been involved. To the best of the authors' knowledge, the research on using CBR to non-crystal materials is exiguous [17,27].

It is fair to say that so far there have been no systematic studies on how to apply CBR based multiscale methods to model amorphous materials, in terms of extrapolating macroscale constitutive relations based on atomistic information. Even though CBR may be a limited approach to model amorphous materials, it might be still useful to utilize its simplicity and low-cost to model amorphous materials. Therefore in this study we hope to examine the possibility as well as limitation on how to use CBR modeling amorphous materials, and compare it with other multiscale methods and the molecular dynamics approach. In particular, based on CBR, we have developed a coarse-grained Parrinello-Rahman (CG-PR) method that is tailored for dealing with complex microstructure of amorphous materials. In this work, we shall mainly focus on how to use the proposed CB-PR method and the multiscale cohesive zone method to model amorphous silicon (a-Si) and Lennard-Jones (L-J) binary glass. This is because that these two models are not only simple enough for the fundamental study, but also are representatives for amorphous materials. Moreover, a-Si is a typical brittle material with prototypical amorphous structure though it may be characterized as a monoatomic material. Furthermore, a-Si is a material that has a great potential for solar cell [28], thin-film transistor [29], flexible display, and many other applications. On the other hand, L-J binary glass is an ideal model for glassy materials with ductility, such as metallic glasses [30,31] and polymer network glasses [32].

The paper is organized in five sections. The simulation methods of MD, coarse-grained Parrinello-Rahman (CG-PR) and MCZM are described in Section 2. Numerical examples are presented in Section 3, in which we compare the simulation results between MD and CG-PR/MCZM for both a-Si solid and L-J binary glass. By analyzing the simulation results, we hope to find a general guideline for application of CBR to amorphous materials. After these examinations, we combined CG-PR method with multiscale cohesive zone model to simulate fracture of amorphous materials, and the simulation results are reported in Section 4. Finally in Section 5, we conclude the study with a few remarks.

2. Simulation methods

In this section, we shall briefly discuss the simulation methodologies that are used in this study, which include: molecular dynamics (MD), the Cauchy-Born based coarse-grained Parrinello-Rahman (CG-PR) method, and the multiscale cohesive zone model (MCZM).

2.1. Molecular dynamics simulation

All MD simulations were carried out by using LAMMPS [33]. Amorphous silicon (a-Si) is modeled by using three body Tersoff potential [34,35] that can be expressed as follows,

$$V_{ij}^{TS} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})]. \tag{1}$$

In the Tersoff potential, the functions f_R, f_A are defined as,

$$f_R(r_{ij}) = A\exp(-\lambda_{ij} r_{ij}); \tag{2}$$

$$f_A(r_{ij}) = -B\exp(-\mu_{ij} r_{ij}), \tag{3}$$

and the cutoff function f_C is defined as,

$$f_C(r_{ij}) = \begin{cases} 1 & r_{ij} \leqslant R_{ij} \\ \frac{1}{2} + \frac{1}{2}\cos\left(\frac{\pi(r_{ij}-R_{ij})}{S_{ij}-R_{ij}}\right) & R_{ij} < r_{ij} < S_{ij} \\ 0 & r_{ij} \geqslant S_{ij} \end{cases}. \tag{4}$$

In order to take into account the three body interaction, the Tersoff potential has a parameter b_{ij} (see Eq. (1)). It explicitly depends on the location of the third atom k, which is expressed as follows,

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{\frac{-1}{2n}} \tag{5}$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) g(\theta_{ijk}) \tag{6}$$

$$g(\theta_{ijk}) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta_{ijk})^2}. \tag{7}$$

For more information on the parameters of the Tersoff potential, readers may consult [35]. In the rest of the paper, we may refer the amorphous silicon as a-Si solid.