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Bridging the length scales through nonlocal hierarchical multiscale modeling scheme

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ABSTRACT

In the current work the nonlocal multiscale bottom-up peridynamic framework is modified (i.e. extended PFHMM) in order to upscale the nonlocally interacting models at different length scales. The generalized scheme was implemented to a complex heterogeneous polymer: ultra high molecular weight polyethylene (UHMWPE). Using extended PFHMM, the atomistic model of UHMWPE was linked with the coarser peridynamic (PD) representative unitcells. Different phases (e.g. highly oriented unidirectional, amorphous or semicrystalline) of UHMWPE were blended during upscaling of polyethylene (PE) microfibrils. In literature, a thorough theoretical investigation on the deformation mechanism of highly oriented UHMWPE microfibrils is not available. So the current work also rigorously discussed the role of different loading conditions (such as torsion, tension and compression), pre-existing damages and aspect ratios on the stiffness as well as the strength of the UHMWPE microfibrils by using molecular dynamics (MD) simulation. Through MD simulation, the effect of complex-loading condition on the strength reduction was also investigated. Cauchy–Born rule was applied through extended PFHMM in order to link the deformation from atomistic scale models with the macroscale UHMWPE representative unitcells. Finally, a slightly modified AIREBO potential was used to show that the unidirectional UHMWPE is independent of strain rate. The results had reasonable agreement with the experimental results. The current work can be considered to be a building block for multiscale modeling of complex heterogeneous materials.

1. Introduction

Over the last decade multiscale modeling has become a very interesting topic within the computational materials science and mechanics community. The fundamental idea of multiscale modeling is to connect different length and time scales (e.g. coupling between atomistic model with a continuum model) in order to extract the information at atomistic scale while the far field boundary condition is applied at the continuum scale. Several works have been done along this direction. In embedded atomistic model the finite element (FE) nodes are linked with the atoms in the handshake region by reducing the degrees of freedom from the atomistic model [1,2]. In quasi-continuum method the concept of Cauchy–Born rule is applied [3]. The deformation gradient from the continuum scale is linked to the representative atoms from the atomistic model. In the bridging method displacements from the atoms are coupled with the FE nodes by interpolation [4]. The hierarchical multiscale model relies on passing information back and forth among different representative volume elements (RVE) at different length scales [5–8]. The generalized mathematical homogenization method (GMH) is applied on the RVE at a certain length scale [5,6]. The N-scale model reduction method is incorporated in the GMH in order to reduce the degrees of freedom. Besides applying FE method as a continuum solver, meshfree methods are also applied at the continuum scale. The necessity of meshfree methods arises when remeshing in FE model becomes expensive. Remeshing is needed for treating elements at significantly different length scales (e.g. crack tip). The common meshfree methods are element free Galerkin method (EFG) [9], radial point interpolation method (RPIM) [10], local radial point interpolation method (LRPIM) [11,12], moving least-square reproducing kernel method (RKPM) [13], smoothed particle hydrodynamics (SPH) [14], material point method (MPM) [15] and peridynamics (PD) [16–18]. Peridynamics is a nonlocal continuum method which uses the governing equations in classical continuum mechanics as integro-differential equations. The nonlocality may be used to develop a multiscale modeling scheme for complex materials. Due to the absence of any local order, multiscale modeling of complex heterogeneous materials is a challenging task. For an example, in amorphous

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polymer the atoms are randomly distributed. During deformation the random spatial arrangement of the atoms evolve. It is a challenging task to keep track of the atoms from polymer and link them with a coarser continuum model. In addition, the atomistic-continuum coupling leads to originate problem regarding spurious wave reflection at the handshake region since the atomistic model is nonlocal and classical continuum model is local. The reflected short wavelength phonon from the atomistic-continuum interface eventually introduces random oscillations in the atomistic domain. It is shown that peridynamics (PD) is analogous to the classical molecular dynamics (MD) formulation as both of the formulations are nonlocal [19,20]. So the issue regarding spurious wave reflection is not a concern. In the current work a peridynamics based hierarchical multiscale modeling scheme (PFHMM) was proposed in order to pass information between PD RVE(s) and atomistic RVE(s) [21,22] without causing any spurious wave reflection [22]. PFHMM possess both top-down and bottom-up information passing schemes. However, it is sometime inevitably challenging to determine the number of PD RVEs at different length scales. Different material has dependency on length scale in a different manner. For amorphous polymers nonlocality at nanoscale exists within a wide range of length scales (e.g. few nanometers). So the molecular interaction among these length scales is very strong compared to macroscale. In the current work the bottom-up PFHMM is modified based on the nonlocality among length scales.

Although PFHMM is generic for any type of amorphous polymers, in the current work we are focusing on multiscale modeling of polyethylene (PE). Based on the manufacturing method PE can be obtained in completely amorphous form or semicrystalline form. Amorphous PE remains in a macromolecule form, known as thermoplastic polymer. PE contains a significant fraction of amorphous phase. Due to the light weight, resistance to chemical reaction, high temperature, etc., PE with different densities are used in wide range of applications. Low density polyethylene (LDPE) possesses less stiffness and strength compared to high density polyethylene (HDPE). Among all types of PE, ultra high molecular weight PE (UHMWPE) has the highest stiffness value (100 GPa) compared to LDPE (0.238 GPa) and HDPE (0.8 GPa). In UHMWPE, the PE chains are highly oriented. This leads to higher stiffness compared to the amorphous PE. UHMWPE single fibers (such as Dyneema SK76) typically consists of a small volume fraction of amorphous phase and a large percentage of crystalline phase. The continuity of the highly oriented PE chains are intermittent [23]. In between continuous fibers there are amorphous PE molecules connecting the highly oriented segments. UHMWPE is widely used in many applications where high performance light weight thermoplastic polymers are used. There are very few works (primarily experimental) available in the literature on mechanical characterization of UHMWPE [23–26]. It is important to develop a theoretical model in order to explore the structural configurations and deformation mechanism of PE at atomistic level and incorporate that into the hierarchical nonlocal multiscale scheme. Similar kind of works have not been noticed in the literature. The current multiscale framework will lead us to capture the deformation and failure of the complex heterogeneous materials (e.g. semicrystalline PE at nanoscale) and pass its effect to the coarser length scale models in the hierarchy in a seamless manner.

2. Peridynamics as a nonlocal continuum theory

The balance equation between rate of change of linear momentum and applied force on a deformable body Ω develops the fundamental equation in classical continuum mechanics is written in Eq. (1) [16–18]

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \nabla\cdot\boldsymbol{\sigma} + \boldsymbol{b}(\boldsymbol{x},t). \tag{1}$$

Here, $\boldsymbol{x}\in\Omega, t$ is the time, ρ is the mass density, $\ddot{\boldsymbol{u}}$ is the acceleration, $\boldsymbol{\sigma}$ is the stress tensor and $\boldsymbol{b}(\boldsymbol{x},t)$ is the body force. This differential equation is not well defined at the discontinuities. The PD formulation introduces integral form of kinematic equation in order to mitigate this issue by calculating the force density on each material point as

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\mathcal{H}}\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})dV_{\xi} + \boldsymbol{b}(\boldsymbol{x},t). \tag{2}$$

In Eq. (2) deformable body $\mathcal{B}$ is represented with respect to an arbitrary frame of reference, $\mathbf{f}$ is the pairwise force applied on particle at $\boldsymbol{x}$ by a neighborhood particle at $\boldsymbol{x}'$ and $\mathcal{H}$ is a spherical region in the neighborhood of $\boldsymbol{x}$ with radius $\delta, \boldsymbol{\xi} = \boldsymbol{x}' - \boldsymbol{x}$ and $\boldsymbol{\eta} = \mathbf{u}(\boldsymbol{x}',t) - \mathbf{u}(\boldsymbol{x},t)$ are relative position and displacement vectors, respectively (Fig. 1). For a certain $\delta > 0$, $\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = 0$ for all $\boldsymbol{\eta}$ when $\|\boldsymbol{\xi}\| > \delta$. This equation may be written more elaborately in terms of bond between $\boldsymbol{x}$ and $\boldsymbol{x}'$ as

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{\mathcal{H}}\{\underline{\mathbf{T}}[\boldsymbol{x},t]\langle\boldsymbol{x}'-\boldsymbol{x}\rangle - \underline{\mathbf{T}}[\boldsymbol{x}',t]\langle\boldsymbol{x}-\boldsymbol{x}'\rangle\}dV_{x'} + \boldsymbol{b}(\boldsymbol{x},t). \tag{3}$$

The peridynamic force state $\underline{\mathbf{T}}[\boldsymbol{x},t]$ is interpreted in terms of mapping the bond between $\boldsymbol{x}$ and $\boldsymbol{x}'$ to a force density per volume which has a cutoff range. Each particle experiences two types of forces: short range forces and long range forces. Short range forces are repulsive in nature. The bond-force on each particle is generated from the bonds it shares with the neighboring particles [16–18].

3. Linking the length scales

3.1. Length scales and nonlocality

The goal in this work is to link the length scales by coarsening through the atomistic to peridynamic models of different sizes. Complex heterogeneous materials have a dependency up to certain length scale. For example, the critical length scale is 30 nm for amorphous polyethylene (PE) [27]. In the amorphous polymers molecules with different lengths coexist. The nonlocal interaction among long chains are different than the one between short chains. As shown in the schematic diagram in Fig. 2(a), the coarser and finer regions in the circle represent molecules with different size and local densities. The nonlocality exists at a same location given that there may be molecules with different characteristic lengths. This creates complexity in the typical coarse graining schemes. Hence, the current work uses the concept of intrinsic hierarchy between atomistic and macroscales.

Within a range of a length scales the stiffness of the Euler–Bernoulli beam varies nonlinearly [28]. It was observed that bending rigidity and the deflection of the beam are significantly dependent on the length scale which was verified by experiments [29,30]. The results showed that the bending rigidity for epoxy decreases exponentially till 100 μm and eventually merges with the prediction from classical theory (i.e. local model). So this indicates that the inhomogeneity in the amorphous materials (within few Å to

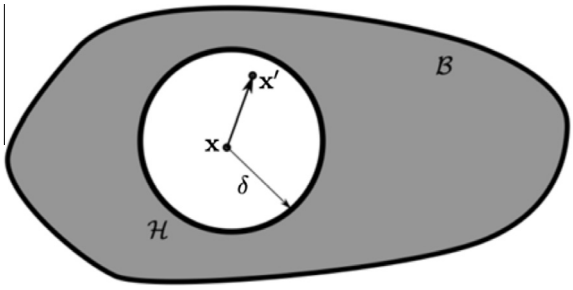

Fig. 1. A schematic diagram of PD model.