International Journal of Solids and Structures 130–131 (2018) 36–48

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

Simulation of micro-scale shear bands using peridynamics with an adaptive dynamic relaxation method

J. Luo[a,*], A. Ramazani[b], V. Sundararaghavan[b]

[a] Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA
[b] Department of Aerospace Engineering, University of Michigan, 1320 Beal Ave, Ann Arbor, MI 48109, USA

ARTICLE INFO

Article history:
Received 1 July 2017
Revised 10 October 2017
Available online 18 October 2017

Keywords:
Microstructure
Crystal plasticity
Peridynamics
Dynamic method
Simulation

ABSTRACT

A peridynamic (PD) implementation of crystal plasticity with an adaptive dynamic relaxation method is presented. Non-ordinary state-based peridynamics and the Newmark's dynamic method with artificial damping are employed to capture strain localizations in polycrystalline microstructures based on a rate-independent crystal plasticity model. Numerical simulations for planar polycrystals are conducted under plane strain pure shear and compression, respectively. The computational efficiency of the explicit PD model is demonstrated to be superior to an implicit PD model for modeling crystal plasticity. The stress field distribution, texture formation, and homogenized stress-strain response predicted by the finite element method and the new dynamic PD model are compared. Finer localization bands are observed in the latter model. The origin and evolution of these shear bands are studied by PD simulations during deformation of three polycrystals with different orientation distributions. Emphasis is placed on the accuracy and efficiency of the adaptive dynamic relaxation method working with crystal plasticity PD models.

1. Introduction

Modeling mechanical behaviors of advanced alloys applied in industrial applications is a persistent and active challenge (Ramazani et al., 2016; Abuzaid et al., 2013; Sun and Sundararaghavan, 2014). One popular numerical model for polycrystalline materials is the crystal plasticity finite element (CPFE) model (Sun and Sundararaghavan, 2014; Roters et al., 2010; Anand and Kothari, 1996) which provides a link between the dislocation-level physics and macro-scale continuum response (Lim et al., 2015). In CPFE models, grains are discretized into finite elements where the crystal plasticity formulations are applied to compute mechanical responses (e.g., stress and strain), crystallographic slip, and reorientation of grains (texturing) at the grain scale (Lim et al., 2015; Roters et al., 2011). However, it is difficult for CPFE models to properly predict strain localizations, in the form of fine shear bands, which have been observed by number of recent experiments (Chen et al., 2017; Khadyko et al., 2016; Pokharel et al., 2014; Kammers and Daly, 2013; Guery et al., 2016). An example of shear band formation in a polycrystal is shown in Fig. 1. The size of shear bands and magnitude of shear computed by standard finite element methods are highly determined by the element size used in the discretization (Pokharel et al., 2014; Kuroda, 2011; Borst et al., 1993).

Considering this disadvantage of CPFE models, different approaches such as non-local constitutive models Evers et al. (2004), higher-gradient models (Menzel and Steinmann, 2000), meshfree methods (Li et al., 2000) have been proposed. Peridynamics, introduced as an alternative integral formulation for continuum mechanics (Silling, 2000), is a particle-based approach capable of handling the formation and propagation of discontinuities. This non-local method, represented by a set of interacting particles, calculates strain at a particle by tracking the motion of surrounding particles. A generalized state-based PD model was later proposed by Silling et al. (2007), in which forces between particles are found using stress tensors obtained from classical constitutive formulations, such as crystal plasticity theory. Recent results based on a crystal plasticity peridynamic (CPPD) model with an implicit Newton–Raphson solver have shown advantages of capturing finer shear bands in planar polycrystals (Sun and Sundararaghavan, 2014).

Implicit methods are traditionally favored compared to explicit dynamic methods for their accuracy at larger time steps (Harewood and McHugh, 2007). However, for crystal plasticity, the computation cost of calculating the tangent modulus matrix is high (Roters et al., 2010). Hence, the new contribution of this paper is a fully explicit implementation of state-based peridynamics for modeling quasi-static deformation of polycrystals. An adaptive dynamic

* Corresponding author.
E-mail addresses: jiangyi@umich.edu (J. Luo), ramazani@umich.edu, ramazani_mat@yahoo.com (A. Ramazani).

https://doi.org/10.1016/j.ijsolstr.2017.10.019
0020-7683/

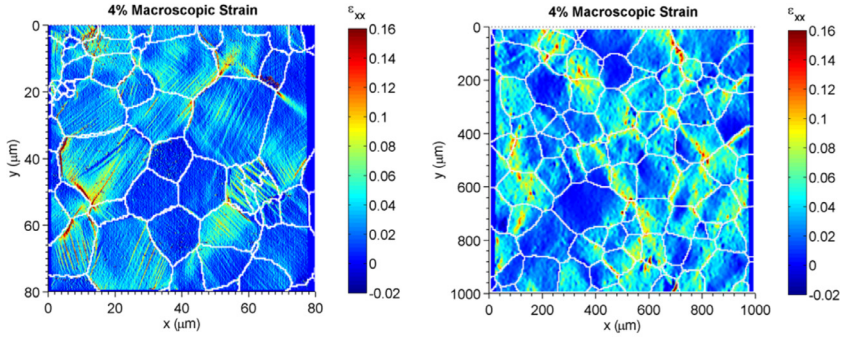

Fig. 1. Tensile strain maps of a magnesium alloy microstructure for two different heat treatments. Experiment data is obtained using the micro-scale digital image correlation technique (Kammers and Daly, 2013). Fine shear bands due to strain localizations are observed in (a).

relaxation method for quasi-static PD simulations as proposed by Kilic and Madenci (2010) is introduced, where an artificial damping ratio estimated from Rayleigh's quotient is selected to dampen the system leading to a steady-state solution. The critical time step is approximated by a numerical analysis of hyperbolic partial differential equations. Accuracy and effectiveness of this new dynamic CPPD model will be demonstrated with numerical examples.

Although peridynamics has been proven powerful in predicting discontinuities and damages (Madenci and Oterkus, 2014; Gerstle, 2015), it still has some intrinsic numerical issues, among which are zero-energy modes and non-trivial treatment of boundary conditions (Breitenfeld et al., 2014; Tupek and Radovitzky, 2014; Wu and Ben, 2015). Recently, different techniques have been applied. For instance, artificial forces are introduced to reduce spurious modes (Breitenfeld et al., 2014); a stabilized PD formulation with mixed local and nonlocal gradient approximations by Wu and Ben (2015) to enhance essential boundary conditions. Moreover, a peridynamic differential operator extending high-order derivatives to their nonlocal forms has been lately proposed by Madenci et al. (2016). Nevertheless, no uniform and standard scheme is employed coefficients or formulations are chosen on a case-by-case basis. With respect to the PD stability issues, simulations in this paper will mostly adopt the smallest horizon radius to better compare with a continuum local CPFE formulation. One special case with an increased horizon length is conducted in a compression test to better analyze the effect of horizon size on characteristic microstructural length scales. Besides, quantities such as deformation gradients are adjusted for smaller horizons at boundary particles in our model.

In the current work, we conduct simulations for planar polycrystalline microstructures under plane strain pure shear and compression, respectively. The numerical efficiency of the explicit method is compared against the previously proposed implicit CPPD method (Sun and Sundararaghavan, 2014) in the case of pure shear. The stress field distribution, texture formation, and homogenized stress-strain response predicted by the classical CPFE model and the new dynamic CPPD model are compared afterwards. In addition, we perform compression tests of three polycrystals with different orientation distributions to study the nature of localization bands identified from the dynamic CPPD method. Section 2 of this paper provides formulations of state-based peridynamics, the adaptive dynamic relaxation method, and their numerical discretization schemes. The crystal plasticity constitutive model and its numerical implementations are given in Section 3. Section 4 compares planar simulations obtained by the explicit dynamic CPPD model with CPFE results, to demonstrate the capability of the new model for capturing finer shear bands in grains. In the last section, a brief summary and some expectations for the future explicit dynamic CPPD model are discussed.

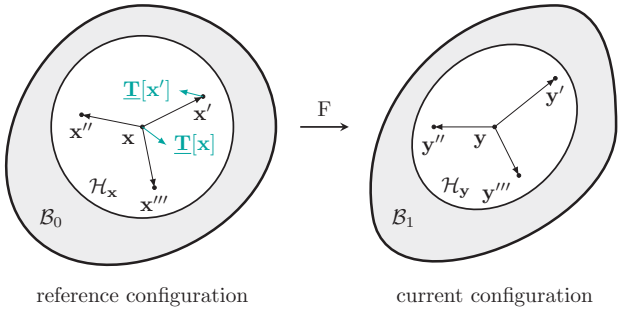

Fig. 2. Kinematics of peridynamics: Particle $\mathbf{x}$ is bonded to all particles ($\mathbf{x}'$, $\mathbf{x}''$, and $\mathbf{x}'''$) within a region $\mathcal{H}_{\mathbf{x}}$. After deformation, particle $\mathbf{x}$ maps to particle $\mathbf{y}$ and the process can be described by an averaged deformation gradient $\mathbf{F}$. $\underline{\mathbf{T}}[\mathbf{x}] = \underline{\mathbf{T}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x}\rangle$ and $\underline{\mathbf{T}}[\mathbf{x}'] = \underline{\mathbf{T}}[\mathbf{x}', t]\langle \mathbf{x} - \mathbf{x}'\rangle$ are force vector states in the reference configuration at particle $\mathbf{x}$ and $\mathbf{x}'$, respectively. In the non-ordinary state-based PD theory, these two force vector states are not necessarily parallel and can be obtained from the classical stress tensor.

2. Peridynamics with an explicit dynamic solver

2.1. State-based peridynamics

The state-based PD model is first presented by (Silling et al., 2007) in 2007, which is a nonlocal integral reformulation of the continuum theory. Consider a material point $\mathbf{x}$ in the reference configuration which can only interact with its neighboring points $\mathbf{x}'$ in a self-center horizon $\mathcal{H}_{\mathbf{x}}$ with a finite radius δ. Given a displacement field $\mathbf{u}$, the current configuration is then represented by $\mathbf{y} = \mathbf{x} + \mathbf{u}$. Let the initial physical domain be $\mathcal{B}_0$ at time $t = 0$ while $\mathcal{B}_1$ is the deformed domain (shown in Fig. 2).

With the introduction of the *deformation vector state* $\underline{\mathbf{Y}} = \underline{\mathbf{Y}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x}\rangle = \mathbf{y}' - \mathbf{y}$, which denotes the deformed state of the bond $\xi = \mathbf{x}' - \mathbf{x}$, the deformation gradient $\mathbf{F}$ at particle $\mathbf{x}$ is reformulated as a nonlocal integration over the horizon:

$$\mathbf{F} = \left(\int_{\mathcal{H}_{\mathbf{x}}} \omega(\underline{\mathbf{Y}} \otimes \xi) dV_{\mathbf{x}'}\right)\mathbf{K}^{-1}, \tag{1}$$

where ω is an *influence function* defined at particle $\mathbf{x}$ in $\mathcal{H}_{\mathbf{x}}$. It weights the influence of each neighbor $\mathbf{x}'$ on the particle $\mathbf{x}$ and can be selected as a spherical function based on the initial bond length, i.e., $\omega = \omega(|\xi|)$. $\mathbf{K}$ is a symmetric shape tensor at particle $\mathbf{x}$, defined as

$$\mathbf{K} = \int_{\mathcal{H}_{\mathbf{x}}} \omega(\xi \otimes \xi) dV_{\mathbf{x}'}. \tag{2}$$