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Atomistic potentials based energy flux integral criterion for dynamic adiabatic shear banding

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ABSTRACT

The energy flux integral criterion based on atomistic potentials within the framework of hyperelasticity–plasticity is proposed for dynamic adiabatic shear banding (ASB). System Helmholtz energy decomposition reveals that the dynamic influence on the integral path dependence is originated from the volumetric strain energy and partial deviatoric strain energy, and the plastic influence only from the rest part of deviatoric strain energy. The concept of critical shear banding energy is suggested for describing the initiation of ASB, which consists of the dynamic recrystallization (DRX) threshold energy and the thermal softening energy. The criterion directly relates energy flux to the basic physical processes that induce shear instability such as dislocation nucleations and multiplications, without introducing ad-hoc parameters in empirical constitutive models. It reduces to the classical path independent J-integral for quasi-static loading and elastic solids. The atomistic-to-continuum multiscale coupling method is used to simulate the initiation of ASB. Atomic configurations indicate that DRX induced microstructural softening may be essential to the dynamic shear localization and hence the initiation of ASB.

1. Introduction

Adiabatic shear banding (ASB) is one of the most important dynamic deformation and failure mechanism of crystalline solids, in which the homogeneous deformation localizes into narrow zones abruptly during a typical short time scale (Bai and Dodd, 1992; Wright, 2002; Molinari et al., 2013). It is widely accepted that the competition between strain hardening and thermal softening dominates the initiation of ASB (Zener and Hollomon, 1944). The initiation mechanism of ASB is rather complex and the understandings still remain unclear.

Osovski et al. (2012b) consider that the microstructural softening due to dynamic recrystallization (DRX), not the thermal softening, may play a key role in dynamic shear localization. DRX precedes and promotes the initiation of ASB, and hence can be regarded as the hint for ASB onset. There are many different criteria on ASB formation, such as the constant dynamic mechanical energy (Rittel et al., 2006), the critical temperature (Medyanik et al., 2007), the critical stress (Batra and Kim, 1992) and the critical strain (Zhou et al., 1996b). These criteria have been successfully adopted in the finite element simulations (Zhou et al., 1996a, 1996b; Medyanik et al., 2007), as well as the meshfree simulations (Li et al., 2001, 2002). Most existing simulation results of ASB initiation and propagation are obtained from continuum computations. Limited to the

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spatial and temporal scale, the initiation of ASB cannot be resolved by molecular dynamics (MD) simulation. Note that, the macro–micro coupling effects are important to the onset of ASB, which need to be investigated theoretically and numerically. Atomistic-to-continuum multiscale coupling methods should be developed to reveal the micro-mechanism of ASB.

The J-integral is a basic analytic tool to study the force on singularities (Eshelby, 1951; Rice, 1968). A unified mechanics analysis of singularity and discontinuity of surfaces can be found (Kosinski, 1986). Early in 1973, Palmer and Rice (1973) use the J-integral as ASB propagation criterion. Zhou et al. (1998) calculate the J-integrals over a series of contours around the tip, and find them to remain constant till the forthcoming of the ASB. In their works, ASB is formulated in the continuum mechanics framework, e.g., it is discontinuity, rather than singularity across the ASB surface. Theoretically, the J-integral will be zero under this assumption, for the total flux of energy toward the tip is zero (Wright and Ravichandran, 1997). However, the J-integral is non-zero in their simulation results. This is because they incorporated the crack model, and the crack model includes singularities. The crack formula in linear elastic fracture mechanics is borrowed to analyze ASB (Palmer and Rice, 1973), and the crack propagates along with the spreading of shear band (Zhou et al., 1998). Dynamic cracking is the outcome of ASB evolution, not its origin, hence the fracture criterion cannot be used directly as the ASB initiation criterion. The formation of ASB is rather complex and the initiation mechanism still remains unclear. In recent experiments, ASB was discovered as the consequence of DRX, dislocations, twins, etc. When DRX occurs, the deformed microstructure is replaced by nucleation and growth of new strain-free grains, together with slip, recovery, grain growth or phase transformation (Osovski et al., 2012a; Dolinski et al., 2010). From this point of view, dynamic ASB can be considered as a highly localized band that consists of multiple singularities. Therefore, it can be studied by using the J-integral.

The J-integral is path independent for quasi-static loading condition and elastic material response, which is unrealistic for the study of dynamic ASB initiation and propagation. The path dependence of J-integral is discussed for elastic–plastic materials (Simha et al., 2008), in which the near-tip J-integral can be calculated from the far-field J-integral and the plasticity influence term. In the review of energy flux integrals for dynamic fracture (Nakamura et al., 1985), the crack tip energy flux can be expressed by the near tip mechanical fields. The J-integral has also been extended to atomistic calculations. The contour integral is evaluated by a total sum of atoms along the specified path in Inoue et al. (1994). This attempt is interesting, but the computation is complicated. Take advantage of the potential energy interpretation, the J-integral is calculated as the potential energy difference between the neighboring crack length in Xu et al. (2004). Though the computational cost has been reduced considerably, the accuracy can hardly be confirmed. Jones and Zimmerman (2010) present a novel methodology. The continuum variable fields in the J-integral are constructed from atomic data. This method is generalized to the finite temperature case (Jones et al., 2011). The difficulties of calculating atomistic J-integral under dynamic loadings lie in two aspects: computational efficiency and path dependence. It should be efficient, consistent, applicable to polycrystals and easy to identify the dynamic and plastic influences to the integral path dependence.

In this paper the atomistic potentials based energy flux criterion in contour integral form is proposed to study the initiation of ASB. In the multiscale hyperelasticity–plasticity constitutive formulation, this energy flux criterion is derived from the embedded-atom method (EAM) potential and the local harmonic approximation in contour integral form, which relates ASB initiation to its underlying physics including the effect of dislocations and phase transformations. Atomistic-to-continuum coupling simulation results indicate that the initiation of dynamic ASB can be well predicted. The main idea is the following: (1) The energy flux integral is deduced from the atomistic potentials, without introducing ad-hoc parameters in constitutive models. The relationship between J-integral and the atomistic scale behaviors can be explored. (2) The integral path dependence is investigated based on the decomposition of system Helmholtz energy. The origin of the dynamic influence and the plastic influence is revealed. The dynamic influence is attributed to the volumetric strain energy and partial deviatoric strain energy, and the plastic influence is governed by the rest part of deviatoric strain energy. (3) The concept of critical shear banding energy is suggested as a quantitative criterion for ASB formation. It is defined to be the energy required for an unit area extension of the shear band. It consists of the DRX threshold energy and the thermal softening energy. (4) The atomistic-to-continuum multiscale coupling method is applied to study the initiation of ASB. The herringbone structure in the band tip, observed from the atomistic simulation results, may exhibit a new shear instability energy dissipation pattern by the propagating dynamic shear band. Atomic configurations indicate that DRX induced microstructural softening may be essential to the shear localization and hence the initiation of ASB, which is confirmed by the experimental evidence in Rittel et al. (2008). The initiation of shear band is predicted by the atomistic potentials based energy flux integral criterion in continuum calculation, and is validated by experimental observations. Once the time scale of MD simulation is enlarged enough to resolve the whole process, the initiation of ASB can be identified from the underlying physics of microstructures, and the critical energy flux calculated from the contour integral can be compared with the experimental result.

Section 2 introduces the basic principles and methods, including the energy flux integral, path dependence analysis in hyperelasticity–plasticity, energy flux criterion, constitutive model and the multiscale method. The results and discussion are given in Section 3, in which the simulation model, energy flux and the micro-mechanism in the initiation of ASB are presented. Section 4 summaries this paper.