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Finite hyperelastic–plastic constitutive equations for atomistic simulation of dynamic ductile fracture

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ABSTRACT

The atomistic-based consistent finite hyperelastic–plastic constitutive (LH) model for multiscale simulation is proposed. The system Helmholtz energy is constructed from an embedded-atom method (EAM) potential with uniformly deformation assumption, which consists two parts: the volumetric part and the deviatoric part. A lattice structure related upscaling strategy is introduced to split the total energy. The volumetric strain energy is used to determine the elastic responses, while the deviatoric strain energy governs the plastic evolution. Based on the maximum plastic dissipation principle and the deviatoric strain energy, we derive the general form of atomistic-based plastic flow rule, which lays the theoretical foundation to build LH model. The evolution equation can be explicitly expressed by the kinematic variables of multiplicative decomposition, which directly relates the flow rule to basic physical processes that induce plasticity such as dislocation multiplications. The isotropic hardening parameters in von Mises yield function are fitted by plastic flow stresses. The integration algorithm of standard finite strain plasticity is developed for LH model. In case of zero deviatoric strain energy, LH model reduces to the classical elastic Cauchy-born (CB) model. Full atomistic simulation of dynamic crack propagation is carried out to validate this model. Plasticity captured by LH model, instead of the elasticity obtained from CB model, is observed after lattice instability, which implies that the ductile fracture can be governed by the collective behaviors of dislocations.

1. Introduction

Recently atomistic-to-continuum coupling multiscale methods have been widely used to study material response at nm–μm length scales. The construction of atomistic consistent and predictive constitutive model remains a long-term challenge for the application of these methods. In the hyperelastic Cauchy-Born (CB) model (Ericksen, 1984), the volume element deforms uniformly as the underlying lattice, hence the macroscopic strain energy can be calculated from the atomistic potential energy. CB model is considered to be consistent with atomistic potential force field, and has been applied to most existing multiscale methods, such as quasicontinuum method (Tadmor et al., 1996), finite temperature quasicontinuum method (Dupuy et al., 2005), bridging scale method (BSM) (Wagner and Liu, 2003), CGMD (Rudd and Broughton, 1998), as well as the interatomic potential finite element method and the lattice dynamical finite element method (Zhong and

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Zhu, 2008; Liu et al., 2010). CB model proved to be accurate under static loading conditions, or before the incipient of lattice instability. However, the nucleation and multiplication of dislocations that triggered by the activation of slip, which eventually leads to the onset of plasticity (Cheung and Yip, 1994; Abraham et al., 2002; Buehler et al., 2003; Buehler et al., 2004), cannot be described by the elastic CB model.

Fundamentals of dislocation induced plasticity are extensively explored based on multiplicative decomposition in Rice (1971), Simo and Ortiz (1985), Moran et al. (1990), Hartley (2003), McDowell (2010) and Clayton et al. (2014). The two-term multiplicative decomposition for elastic–plastic crystals is first formulated by Bilby et al. (1957), in which the total deformation gradient is decomposed into the elastic component and the plastic component. The elastic component is caused by stretching and rotation of the crystal lattice (volumetric). Plastic component results from dislocation motions and is defined as lattice-preserving or lattice invariant, since dislocation glide is volume-preserving (Clayton, 2011). The three-term decomposition is proposed for elastoplasticity of polycrystals in Clayton and McDowell (2003), and Clayton et al. (2014) reveals that the third term, e.g., the local component of lattice deformation, is significant in cases of large defect densities. Based on the concurrent atomistic continuum (CAC) methodology, key phenomena of dislocation dynamics, including dislocation migration and formation of intrinsic stacking faults, can be captured by the coarse-grained atomistic simulations in Xiong et al. (2012). For thermally-activated dislocation motion and generation, Bammann and Solanki (2010) presents a new consistent polycrystalline elastoplasticity model, which coupling kinematics and thermodynamics with damage. Moreover, Homayonifar and Mosler (2011) and Homayonifar and Mosler (2012) demonstrates the dislocation slip and microstructure evolution in magnesium by crystal plasticity theory.

Successful implementations of multiplicative decomposition have also been witnessed in finite hyperelastic–plastic constitutive models. The associative flow rule can be deduced with the maximum plastic dissipation principle (Hill, 1983), and Simo (1988) generalized it to the hyperelastic framework. In the newly developed finite strain kinematic hardening constitutive models, the plastic evolution is derived from the generalized normality rule (Badreddine et al., 2010), or the structure tensors (Vladimirov et al., 2010). Temperature effects are coupled in the plastic evolution by Ghavam and Naghdabadi (2011), in which the flow stress is dependent on the temperature and strain rate, and thermally activated damage is incorporated to account for the physical mechanisms of failure by Vignjevic et al. (2012). Combining the isotropic Helmholtz strain energy and irreversible thermodynamics, the phenomenological constitutive models have been developed for shape memory alloys (Arghavani et al., 2010; Arghavania et al., 2011).

However, to construct an atomistic-to-continuum coupling multiscale constitutive model, three conditions are necessary. First, consists with the underlying lattice. Second, plasticity is reasonably described and easily apply to the existing macro solvers of multiscale methods. Finally, includes dislocation effects. To some extent, it is the plastic extending of CB model. Moreover, the associative flow rule should be deduced from the interatomic potential energy in hyperelastic framework with multiplicative decomposition.

An atomistic-based finite hyperelastic–plastic (lattice hyperelastic, LH) constitutive model is built for studying dynamic ductile fractures in this manuscript. It also suggests a new way to construct macro–micro consistent hyperelastic–plastic constitutive equations, which is a bottleneck in the development of atomistic-to-continuum multiscale methods. The basic ideas are: (1) Energy splitting. The system Helmholtz energy that constructed from an EAM potential with uniformly deformation assumption consists two parts: the volumetric part and the deviatoric part. A lattice structure related upscaling strategy is introduced to split the total energy. The volumetric part is supposed to be stored in the elastic deformation, and is determined by the upscaled elastic Green's strain tensor and the underlying lattice structure. The deviatoric part is the outcome of atomic bonds breaking and dislocation motions. (2) Plastic evolution. The associative plastic flow is derived based on the deviatoric strain energy and the principle of maximum plastic dissipation. With the kinematic relationships of the deviatoric functional, the proof of the atomistic-based plastic flow rule is provided for general Helmholtz energy, which is the theoretical foundation for building LH model. The evolution equation can be explicitly expressed by the kinematic variables of multiplicative decomposition. Plasticity of the volume elements is viewed as the consequence of multiplication of glide dislocations, without tracking each individual dislocations or grains. Related integration algorithm is developed, and material frame indifference is ensured by using tensorial transformations (Simo and Hughes, 1998). (3) Yield function. Von Mises yield condition with isotropic hardening function is adopted in the plastic evolution computation. Yield strength and hardening moduli of yield function are fitted by the flow stresses in crystal plasticity, since empirical formula for this scale is unavailable. By this way the effects of dislocations are embedded into von Mises yield function for LH model. If there is no plastic flux, e.g., the deviatoric part of the potential energy is zero, LH model will acquire the same result as that of the CB model. At last, numerical experiments of crack propagation are carried out to validate LH model, by comparing with CB model and full atomistic simulations. The effects of dislocation interactions, e.g., atomic plasticity (Buehler et al., 2004), can be observed from LH model before fracture.

The paper is organized as follows: the hyperelastic–plastic LH model is proposed in Section 2, including the governing equation, multiplicative decomposition with energy splitting and derivation of associative flow rule. Numerical aspects are presented in Section 3, consists local integration algorithm, yield model and finite element method. Simulation results and discussions are presented in Section 4, and Section 5 summaries this paper with concluding remarks. The proof of lemma in Section 2 is provided in Appendix A. The methods for computing deviatoric strain energy are introduced in Appendix B.