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Smoothing technique based crystal plasticity finite element modeling of crystalline materials

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ABSTRACT

The smoothed finite element method (S-FEM) is known for its outstanding performance for solid mechanics problems, and working effectively with triangular or tetrahedral mesh that can be generated automatically for complicated geometries. In this work, a framework of S-FEM for modeling anisotropic crystalline plasticity is presented to simulate the mechanical behavior with rate-independence. The strain smoothing technique is extended to deal with finite strains in a nonlinear incremental integration procedure based on the Newton–Raphson scheme. The constitutive model utilizes a hyperelastic-based multiplicative plasticity method, which involves a local multiplicative decomposition of the deformation gradient into an elastic and a plastic part. The stress updates for a planar double-slip model exploit the return-mapping method with exponential map algorithm. The capability of the simulations to capture the strain localization and to handle plastic incompressibility of single crystal are demonstrated in representative examples. The proposed formulations and algorithms are also implemented to explore the mesoscopic and macroscopic elasto-plastic behavior of polycrystalline aggregates through modeling the synthetic microstructure constructed by Voronoi tessellation technique.

1. Introduction

In crystals, the mechanical behaviors are essentially anisotropic, i.e., mechanical properties such as plastic deformation are direction dependent. Microscopically, the properties of anisotropy are related to forming a crystalline structure (lattices) with certain specific, characteristic orientations during crystallization, and in reality a variety of crystallographic defects such as twins, and dislocations or stacking faults. The continuum crystal plasticity includes considerable models to cope with the anisotropic deformation of crystals, developed since the contributions of pioneers such as Sachs (1928) and Taylor (1938).

Over the past three decades, a large class of research has been conducted to describe the constitutive and numerical aspects for both single crystals (monocrystals) and polycrystals. The numerically tractable constitutive models, incorporating existing knowledge of the physics of crystal deformation and continuum, were invented to tackle crystal mechanical problems subjected to complicated internal and/or external boundary conditions. For single crystal, one of the most used numerical tools is the crystal plasticity finite element method (CPFEM). This method is used with various models and was proposed to study the anisotropic plastic behavior by many investigators (Mandel, 1973; Peirce et al., 1982, 1983; Asaro, 1983; Asaro

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and Needleman, 1985; Havner, 1992; Rashid and Nemat-Nasser, 1992; Borja and Wren, 1993; Miehe, 1996a,b; Steinmann and Stein, 1996). Some critical analysis of behaviors predicted from these models and new explorations can be found in literature (e.g., Busso and Cailletaud, 2005; Ling et al., 2005; Kuchnicki et al., 2006; Li et al., 2008; Kuroda, 2011; Anand et al., 2012; Niordson and Kysar, 2014; Bargmann et al., 2014). Generally, CPFEM evolves the equilibrium of the forces and the compatibility of the displacements based on a weak form of the principle of virtual work, with certain crystal plasticity constitutive laws. CPFEM models possess many advantages, including their capability to describe the inelastic deformation and localization processes by encompassing various constitutive formulations for plastic flow and hardening at microscopic crystallographic sliding level, even for complicated geometry or boundary conditions.

Crystal plasticity can also be exploited to study material behaviors of polycrystals from the behavior of individual grains. The reason is that polycrystals are assemblies of large numbers of single crystals (grains), each of which can deform by crystallographic slip with varying orientations. As such, the actual solution of a problem of the macroscopic behaviors of a polycrystal may be a highly complex elastic–plastic boundary value problem for a crowd of anisotropic, continuous and fully contiguous crystallites (Asaro and Lubarda, 2006). To deal with the polycrystal plasticity, a classical approach is to average the crystal interactions to describe macroscopic behavior. An early attempt is to assume that all grains experience the same state of stress so that it satisfies the equilibrium condition across the grain boundaries but violates the compatibility conditions (Sachs, 1928). The Taylor model (Taylor, 1938) assumes that grains within the aggregate experience the same state of deformation so as to ensure the compatibility conditions, however the equilibrium condition is neglected. To satisfy both compatibility and equilibrium conditions across the grain boundaries, a self-consistent model was first constructed by Kröner (1958) and then further extended (Budiansky and Wu, 1961; Hill, 1965; Hutchinson, 1970; DeBotton and Castaneda, 1995; Segurado et al., 2012). In a self-consistent model, each grain is modeled as an inclusion embedded in a homogeneous matrix of surrounding material maintaining mechanical properties of the polycrystal. A number of investigations with new models have been conducted to link the grain level mechanical response to the response of a polycrystalline aggregate including developing a constrained hybrid model (Parks and Ahzi, 1990), generalized Taylor models (Asaro, 1983; Asaro and Needleman, 1985; Mathur et al., 1990; Kalidindi and Anand, 1992; Habraken and Duchêne, 2004) and Greens function fast Fourier transform (FFT) models (Lebensohn et al., 2012; Eisenlohr et al., 2013), constructing dislocation density-based crystal constitutive equations (Lee et al., 2010), application of statistical continuum mechanics to study polycrystals (Garmestani et al., 2001; Zhang et al., 2011), and so on. Due to the development of computing power over the last few decades, many crystal plasticity models have been integrated into FE simulation tools and successfully applied to numerous practical problems (e.g., Watanabe and Terada, 2010; Kim et al., 2013). To reduce the CPU time involved in crystal plasticity simulations (especially for large grain assemblies), some computationally efficient strategies have been proposed recently (e.g., Rousselier and Leclercq, 2006; Mahesh, 2010; Knezevic and Savage, 2014; Knezevic et al., 2014). So far, crystal plasticity models based on FE simulations are able to effectively model polycrystals at both microscopic and macroscopic scales. On topics related to kinematics, homogenization and multiscale methods, one can refer to the latest review paper (Roters et al., 2010).

In CPFEM simulations, especially in modeling of polycrystal deformation, the mesh discretization for a domain with a great quantity of grains needs careful consideration. To discretize a domain with internal grain boundaries, the T-mesh (using triangular elements for 2D or tetrahedral elements for 3D) is always easy to generate compared to other mesh types (e.g., quadrilateral mesh for 2D or hexahedral mesh for 3D). However, the conventional FEM models using T-mesh often suffer from poor accuracy, excessive stiffness in shearing/bending, sensitivity of mesh distortion and sometimes rigid behavior of entire mesh, etc. In addition, because of the plastic incompressibility of (single) crystals, an appropriate numerical technique, which can deal with volumetric locking phenomena, is very necessary. Fortunately, the recently proposed smoothed finite element methods (S-FEM) can achieve higher accuracy than the commonly used low order FEM (Liu et al., 2007). S-FEM was proposed as a special linear version of smoothed point interpolation methods, theoretically founded by the generalized smoothed Galerkin weak form (it can be named as weakened weak form, or W2 form) on G space theory (Liu, 2010). The essential idea in the S-FEM is to utilize a standard finite element background mesh (in particular T-mesh) and associated smoothed strain field to build numerical models with good performance (Liu and Trung, 2010). Other than element based implementation in the standard FEM, the S-FEM techniques implement and evaluate the weak form based on smoothing domains. Such an implementation in S-FEM can be located within the elements but more often beyond the elements that brings in the information from the adjacent elements. As a result, a number of different S-FEM methods were proposed by various fashions of construction of smoothing domains, such as CS-FEM, NS-FEM, ES-FEM and FS-FEM (e.g., Liu et al., 2007, 2013, 2009a,b; Zeng et al., 2013; Nguyen-Thoi et al., 2009). And the strain field has naturally satisfied certain conditions such as linear independence to guarantee the stability and convergence for W2 scheme.

Compared to the standard linear displacement finite element method (LFEM), S-FEM can overcome some inherited drawbacks observed in LFEM, such as stress inaccuracy (Liu et al., 2010), sensitivity to element distortion (Dai and Liu, 2007), and volumetric locking phenomena (Nguyen-Xuan et al., 2010; Chen et al., 2012). A summary of major properties of S-FEM can be found in Liu and Trung, 2010. It can be seen that the class of S-FEMs has become a practical and effective tool for analysis of various types of solid mechanics problems. Among these S-FEM models, the ES-FEM was found to be the most computationally efficient (Nguyen-Xuan et al., 2013). Based on those good features (e.g., high accuracy and convergence rates, mesh distortion immunity as absence of isoparametric mapping and volumetric locking free) already obtained for ES-FEM so far, we attempt to extend it into crystal plasticity modeling. In this work, we present the formulation and numerical implementation of a hyperelastic-based multiplicative plasticity constitutive model based on the ES-FEM scheme to describe the