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Crystal plasticity extended models based on thermal mechanism and damage functions: Application to multiscale modeling of aluminum alloy tensile behavior

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ABSTRACT

The mechanical anisotropic properties of aluminum alloy are studied using multi-level approaches for strain-rate and temperature-sensitive large plastic deformation of polycrystalline aggregates. Unlike previous researches, the thermal effect and the damage evolution process are considered simultaneously and integrated in the CPFEM method. In the microscopic constitutive equation of crystal plasticity, the shear strain rate on the slip system is described by an advanced exponential function based on thermal activated mechanism, instead of traditional phenomenological power-law function. To determine the rate-sensitive material parameters in this new model, the strain rate and temperature jump tests are performed. In addition, a simulation of one representative volume element is compared to the results of conventional tensile tests to obtain other thermal parameters. Coupled with the continuum damage evolution formula, this thermal affected crystal plasticity model is then implemented in a single crystal analysis for different orientation, temperature and strain rate conditions. Finally, this extended crystal plasticity model is applied in the finite element method to simulate the mechanical properties of 5052 aluminum alloy at absolute temperature 473 K. Taylor model is also used to compare these simulations as well as the experimental data. The results show that the damage model coupled in the crystal plasticity is able to predict the mechanical response of 5052 aluminum alloy; moreover, this model can simulate the explicit evolution of damage factor and local stress concentration in the deformation of standard tensile test specimen. In the simulation, the specimen is meshed by rectangular elements and each element is given an initial orientation at the first time increment step. This study argues that even in high temperature, the orientation mismatch between adjacent grains could lead to early cavity or crack initiation and the damage development is similar to the void evolution theory. An explanation of the possible fracture angle is given in the thermal tensile test due to polycrystalline anisotropy. At last, the analysis of stress heterogeneity and texture evolution is also shown in this study.

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1. Introduction

Aluminum based alloys (AA) are widely used in vehicle industry, especially as structural components such as door, trunk and other body panels, bumper, engine hood. In new transportation design, AA replacing steel are effective materials for reduction of both the vehicle weight and the CO_2 emission ratio because of their high specific strength and excellent corrosion resistance (Toros et al., 2008). It has been proved that an experimental–numerical approach is applicable and efficient in studying ductile facture (Pedersen et al., 2015), strain rate and temperature effect (Mahabunphachai and Koç, 2010; Toros and Ozturk, 2010; Khan and Baig, 2011; Kabirian et al., 2014; Chen et al., 2015a,b) on AA tensile behavior. However, previous models are mostly phenomenological and lack of metallographic essential relations between microstructure evolving and mechanical response. In AA thermomechanical process, dynamic recrystallization is simulated using continuum mechanics crystal plasticity model (Sidor et al., 2011) and Monte Carlo algorithm (Sepehrband et al., 2015). In the fatigue damage evaluation of AA, three current models, Elber, Walker and unified approach have been applied to simulate the fatigue crack (Duran and Hernandez, 2015) and a modified plastic strain energy approach is used to prediction damage under thermal and mechanical fatigue loading (Azadi et al., 2015).

For the purpose of research on metallurgical deformation mechanism of AA, the anisotropic plastic behavior should be considered as the primary issue in crystallography. As a result of crystallographic anisotropy, many associated macroscopic phenomenon including material strength, strain hardening, crack and damage are orientation dependent (Tasan et al., 2014; Kim and Yoon, 2015; Khan et al., 2015). These macro-mechanical behaviors are mostly due to superposition of the single crystal elastic–plastic anisotropic properties. In this case, multi-level scale methods are developed and early mean-field polycrystalline schemes of describing this directional property such as Taylor, Saches and Bishop-Hill and Kroner are applied to simple boundary conditions (Sarma and Zacharia, 1999; Miehe et al., 1999). In these codes, homogenization of stress or strain field in single crystal could explain some texture evolution using polar diagram, however, the co-deformation effects at grain boundaries on lattice reorientation were not revealed explicitly. As the finite element method approximation since 1980s, a new method called crystal plasticity extended finite element method (CPFEM) is proposed and brought into the crystal mechanics modelling to take inner interactivity and complicated outer boundary condition into account (Roters et al., 2010; Knezevic et al., 2009; Chen et al., 2015a,b). Here in this study, the Taylor model is implemented to predict the macro-mechanical response in tensile deformation in order to compare with CPFEM results. An advanced spectral Taylor model is studied in 2008 (Knezevic et al., 2008), which involves a local spectral interpolation using discrete Fourier transform (DFT) method and achieves a high computational efficiency with irreducible precision. In three-dimensional (3D) framework, the stress or strain heterogeneity and plastic deformation near grain boundaries could be better understood using CPFEM. Combined with discrete Green's function fast Fourier transform (FFT) and spectral interpolation, CPFEM can potentially efficiently and accurately simulate the orientation-dependent mechanism at the grain interface (Eisenlohr et al., 2013; Lebensohn et al., 2012). Grain interactions are modeled and neighbor effects on co-deformation are well captured directly on the local stress and strain fields at grain boundaries (Knezevic et al., 2014) and phase interfaces (Ardeljan et al., 2015) in 3D CPFEM model. Theoretically, each scale of CPFEM is hierarchically incorporated by developing various constitutive models which account for microstructure-property relations (Gawad et al., 2015; Zhang et al., 2014a,b, 2015). For example, dislocation density based constitutive model (Knezevic et al., 2013a,b; Kitayama et al., 2013; Zecevic and Knezevic, 2015; Knezevic et al., 2016) has been confirmed to describe the deformation of polycrystalline aggregates dependent on the mechanical loading and strain path changes. Recent years, a few researches have applied CPFEM to two-phase systems to show co-deforming process near phase interface (Mayeur et al., 2013; Mayeur et al., 2015; Hansen et al., 2013; Ardeljan et al., 2014). These CPFEM simulations focus on the small scale and the finite element mesh size is equivalent to or even smaller than the real grain size, so that the stress heterogeneity and strain localization, even initial crack near grain boundaries could be revealed by microstructural mismatch among grains.

Considering more complex imposed conditions such as temperature and strain-rate effects on plastic behavior of materials using CPFEM, most researches have been concentrating on modifying and constructing the constitutive relations of anisotropic single crystal and polycrystal (Knezevic et al., 2013a,b; Siddiq and Sayed, 2012; Libert et al., 2011; Khan et al., 2012; Pandey et al., 2013). In order to describe the thermal affected microscopic deformation on the slip system, many phenomenological equations, including Hollomon (power-law), Ludwik, Ghosh and Swift models, are generally used to develop the constitutive theory. The metallurgical and mechanical variables become the functions of constitutive parameters with interpolation of present temperature, strain rate and microstructural orientation of polycrystalline grains. Logé and Chastel (2006) proposed an early approach of thermal-mechanical coupling, and the thermal strain rate is considered in division of total strain rate and also several metallurgic phenomenon are shown including thermal dilatation and phase transformation plasticity. Knezevic et al. (2013a) have applied a visco-plastic self-consistent model (VPSC) is to homogenization of the large scale polycrystal and to calculation of the polycrystalline texture behavior as a function of strain rate and temperature. In their study, one crystal is related to one representative volume element (RVE) and the grain number is large enough to study the texture evolution. As one of the advanced mean-field polycrystalline scheme compared to Taylor or Saches model, however, VPSC is still not capable of capturing the interactions among grains which may affect the orientation distribution and mechanical behavior. In view of the spatial local strain and stress field distribution inside polycrystal, 3D CPFEM framework is introduced, and the resolved shear stress on the slip system are built as functions of dislocation dynamics and temperature variation in, which indicates that heterogeneity increase with temperature (Libert et al., 2011). Arising from thermo-mechanical coupling, temperature field evolution in plastic deformation of metals is calculated involving heat generation of

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