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Predicting plastic flow and irradiation hardening of iron single crystal with mechanism-based continuum dislocation dynamics

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ABSTRACT

Continuum dislocation dynamics (CDD) with a novel constitutive law based on dislocation density evolution mechanisms was developed to investigate the deformation behaviors of single crystals. The dislocation density evolution law in this model is mechanism-based, with parameters predicted by lower-length scale models or measured from experiments, not an empirical law with parameters back-fitted from the flow curves. Applied on iron single crystal, this model was validated by experimental data and compared with traditional single crystal constitutive models using a Hutchinson-type hardening law or a dislocation-based hardening law. The CDD model demonstrated higher fidelity than other constitutive models when anisotropic single crystal deformation behaviors were investigated. The traditional Hutchinson type hardening laws and other constitutive laws based on a Kocks formulated dislocation density evolution law will only succeed in a limited number of loading directions. The main advantage of CDD is the novel physics-based dislocation density evolution laws in describing the meso-scale microstructure evolution. Another advantage of CDD is on cross-slip, which is very important when loading conditions activate only one primary slip system. In addition to the dislocation hardening, CDD also takes into consideration dislocation defect interactions. Irradiation hardening of iron single crystal was simulated with validation from experimental results.

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1. Introduction

Mechanical behavior simulations of polycrystalline materials are established on single crystal plasticity constitutive models based on slip system activity. In earlier treatments, the elastic–plastic formulations developed since the 1960s are strain rate independent (Asaro and Rice, 1977; Hill, 1966; Mandel, 1965; Simo and Taylor, 1985) with yield surface defined by Hill's criterion. Later, a viscoplastic approach was proposed to achieve unique solutions to avoid the numerical multiple solutions from using strain rate sensitivity formulations (Asaro and Needleman, 1985; Hutchinson, 1976; Peirce et al., 1982). The essence of viscoplasticity theory is the hardening law, usually in a power law format, to relate the shear stress in each slip system to the shear strain rate. The advantage of the power law formulation is due to the derivation of viscoplastic potential with the capability to capture saturation effect at a high strain rate. Different versions of isotropic and anisotropic viscoplastic constitutive theories have been developed. Examples include MATMOD equations proposed by Henshall (1996) and Miller (1976) to describe viscoplasticity function as a combination of a hyperbolic sine function and a power function. Limited to small strain, back stress is used for kinematic hardening and a drag stress for isotropic hardening. Another example is

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Robinson's formulation, which is more complicated, using a back-stress, a drag stress, a yield stress, and a power function for the viscoplastic flow (Arnold and Saleeb, 1994). There are many other versions taking into consideration different factors. With the development of the theory of slip systems, hardening is decomposed into two parts: latent hardening and self hardening, both in the exponential function form to describe interaction between different slip systems (Asaro, 1983; Asaro and Needleman, 1985; Peirce et al., 1982). Nevertheless, most theories of resistance of shear stress evolution are empirical with the parameters determined by fitting the model to the experimental stress strain curves.

With the advent of dislocation dynamics and multiscale modeling, alternative constitutive laws were proposed to introduce the knowledge generated from dislocation theory to the continuum plasticity framework. For example, (Zbib and Diaz de la Rubia, 2002; Devincre et al., 2008; Groh et al., 2009; Alankar et al., 2012b) proposed multiscale approaches to establish a dislocation-based continuum model to incorporate discrete and intermittent aspects of plastic flows. In these approaches, strain hardening can be predicted through the modeling of mean free paths of dislocations. Other statistical aspects from dislocation dynamics simulation, such as dislocation densities, are used as internal state variables to capture deformation behavior of single crystals (Arsenlis and Parks, 2002; Ortiz et al., 2000). Another front noteworthy is Sandfeld's work (Hochrainer et al., 2007; Sandfeld et al., 2011) to bridge statistical continuum mechanics with dislocation dynamics by dislocation density tensor. Using a statistical description of dislocation interactions in terms of a Taylor-type yield stress and a back stress, which describes short-range repulsion of dislocations of the same sign, key features from discrete dislocation dynamics simulations were captured. The core of the interaction between the discrete dislocation dynamics and crystal plasticity is the evolution law of dislocation density.

In this study, we develop a continuum dislocation dynamics (CDD) model with mechanism-based dislocation density evolution laws. The advantage of this physics-based model is demonstrated by comparing it with the traditional single crystal constitutive equation using Asaro's hardening law (SCCE-T) and the dislocation density-based single crystal constitutive equation (SCCE-D) proposed by Wagoner et al. (Lee et al., 2010a; Lim et al., 2011). Further, the CDD model is applied to simulate the irradiation hardening and validated by experimental data on iron single crystals. The success of CDD will find broad application in mechanical behavior of polycrystalline structural materials under different loading conditions and severe environments. The development of new-generation nuclear reactors depends on the availability of materials that can operate safely in severe environments for an extended service lifetime (Forum, 2002; Guerin et al., 2009). Materials operating in such a harsh environment are subjected to high doses of irradiation which causes changes in microstructure. These changes are responsible for dimensional instabilities, such as swelling and irradiation creep, and mechanical property evolution and degradation, such as irradiation hardening and post-yield deformation behavior including plastic flow and subsequent localization, which impact component performance and reliability.

Current models that address the issue of defect production and interaction are limited to one scale only, with limited interactions between the different scales. At the smallest scales (nanometer and picoseconds), irradiation dose and temperature cause the coalescence of vacancies and interstitials into voids and dislocation loops. These defects and clusters diffuse over macroscopic length and time scales, significantly altering the chemistry and microstructure of the material. Discrete dislocation dynamics (DDD) is a powerful tool that has been advanced significantly in the past decade (Canova et al., 1993; Ghoniem and Sun, 1999; Tschopp and McDowell, 2008; Zbib et al., 1996, 1998). It has been used to explain the effect of irradiation on mechanical properties through large-scale simulations of interaction of numerous numbers of dislocations with defect clusters. The work of Zbib and co-worker have shown that dislocations interactions with the elastic fields of nano-sized defect clusters in Cu and Pd lead to hardening followed by localized deformation and channel formation resulting from defect cluster annihilation by dislocations (Diaz de la Rubia et al., 2000; Ghoniem et al., 2000; Hiratani et al., 2002a,b; Khraishi et al., 2002a; Li et al., 2010; Zbib et al., 2000).

The goal of this study is to predict the stress–strain curve and the critical resolved shear stress as a function of defect density, which is then used in the crystal plasticity model. However, in order for this method to work, a detailed knowledge of the dislocation mobility in an analytical form inside the materials is required. To effectively predict the mechanical behavior of the materials under irradiation at the continuum scale, critical information should be determined and progressively passed from one scale to another.

As shown in Fig. 1, molecular dynamics is first used to calculate dislocation mobility as a function of temperature and alloy composition in a suitable form for the dislocation dynamics framework. The results gathered from the DDD simulations then lead to the evaluation of the dislocation density and critical resolved shear stress in iron single crystal as well as irradiation damage. Finally, the dislocation density evolution law obtained from DDD is used in CDD for mechanical behavior prediction.

2. Physics based continuum dislocation dynamics

The CDD framework uses the principle of crystal plasticity and was improved by introducing more physics-based mechanisms to substitute empirically derived constitutive and hardening laws. Based on the traditional kinematics of crystal

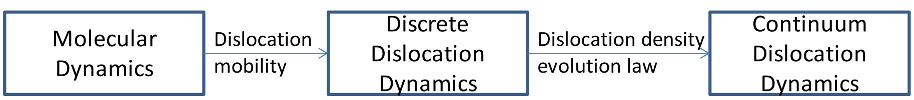

Fig. 1. Scheme of multiscale approach in mechanical flow prediction.