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A numerical procedure enabling accurate descriptions of strain rate-sensitive flow of polycrystals within crystal visco-plasticity theory

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Highlights

- A method enabling crystal visco-plasticity to consider realistic rate-sensitivity exponents is developed.
- The method separates constant structure (the exponent) from evolving structure (the activation stress) rate-sensitivity.
- The method within VPSC is applied to simulate strain rate-sensitive deformation of Cu from 10^{-4}/s to 10^{4}/s.
- The method does not increase the computation time involved in polycrystal simulations.

Abstract

The plastic deformation of polycrystalline metals is carried by the motion of dislocations on specific crystallographic glide planes. According to the thermodynamics theory of slip, in the regime of strain rates, roughly from 10^{-5}/s to 10^{5}/s, dislocation motion is thermally activated. Dislocations must overcome barriers in order to move, and this concept defines critical activation stresses τ_c^s on a slip system s that evolve as a function of strain rate and temperature. The fundamental flow rule in crystal visco-plasticity theory that involves τ_c^s in order to activate slip has a power-law form: $\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{|\tau^s|}{\tau_c^s}\right)^n sign\left(\tau^s\right)$. This form is desirable because it provides uniqueness of solution for the active slip systems that accommodate an imposed strain rate; however, it also introduces a strain rate dependence, which in order to represent the actual behavior of polycrystalline materials deforming in relevant conditions of temperature and strain-rate usually needs to be described by a high value of the exponent n. However, since until now the highest value of n was limited by numerical tractability, the use of the power-law flow rule frequently introduced an artificially high rate-sensitivity. All prior efforts to correct this extraneous rate sensitivity have only lessened its effect and unfortunately also at the expense of substantial increases in computation time. To this day, a solution for the power-law exponent reflecting true material behavior is still sought. This article provides a novel method enabling the use of realistic material strain rate-sensitivity exponents to be used within the crystal visco-plasticity theory without increasing computation time involved

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in polycrystal simulations. Calculations are performed for polycrystalline pure Cu and excellent agreement with experimental measurement is demonstrated.

Keywords: Dislocations; Microstructure; Crystal plasticity; Rate-dependent material; Numerical methods

1. Introduction

Much of the physics of plastic deformation and the role of dislocation motion in it were known before the development of crystal plasticity based models. Dislocation glide marks over polished and deformed surfaces of metallic samples were reported before 1900 [1,2]. It was then concluded that dislocation glide on specific crystallographic planes and directions lying on those planes and their glide imparts the needed shear to deform the crystal. It was also observed that not all crystallographically equivalent planes and directions in a crystal were active during plastic deformation.

Later, the theory of the thermodynamics of slip was developed. It builds on the idea that dislocation motion is thermally activated in the strain rate ranging roughly from 10^{-5}/s to 10^{5}/s [3,4]. The critical stress τ_c^s to move dislocations on an individual system is generally comprised of two components. The first is an intrinsic athermal stress, representing lattice friction and hence thought not to depend on strain rate within the aforementioned thermally activated regime. The second is a dislocation-interaction term, which is controlled by overcoming obstacles on the glide plane, such as other intersecting dislocations, and would generally depend on both strain rate and temperature. τ_c^s depends on chemical composition and evolves as the microstructure within the grain evolves, which includes for instance, dislocation storage, twinning, and substructure development [5–9]. This rate-sensitive dislocation motion occurs within every plastically deforming crystal in the polycrystalline aggregate and causes the macroscopic flow stress–strain response of the polycrystal to depend strongly on the applied stress, strain rate, and temperature of deformation [10,11]. A current overarching aim of materials modeling is to relate the rate-sensitive motion of dislocations to the deformation of a crystal or set of crystals when strained at a particular temperature and strain rate.

An essential and critical part of this modeling effort is the adoption of a sound criterion (or criteria) for activating crystallographic slip. However, the fact that crystal deformation generally involves slip on more than one slip system makes this a challenging task. Most pure metals with a face centered cubic crystal structure (e.g., Cu, Ni, Al) deform on one slip family $\{111\}\,\langle 1\bar{1}0\rangle$, which contains twelve independently oriented slip systems [12–14]. Metals, such as steel and most of refractory metals, with a body-centered cubic crystal structure, have two or three families, making up 24 or 48 slip systems [15–19]. Metals with a lower symmetry crystal structure, like hexagonal close packed Mg, Zr, Be, or Ti metals or orthorhombic U, possess an even larger suite of slip families and systems [20–25]. When plastically deformed, a crystal accommodates strain using a small subset of these systems. Which systems are activated, how many, and the distribution of shear among them are collectively referred to as slip activity.

Predicting slip activity is fundamental to be able to predict the reorientations of the crystals and material flow stress with strain. The theory of crystal plasticity can predict slip activity and relate it to the geometry of crystal deformation; however, it still requires a separate and basic criterion for activating an individual slip system. All polycrystal plasticity based constitutive models, ranging from mean-field models, such as the upper bound Taylor model [26], lower bound Sachs model [27], and the various self-consistent schemes, such as visco-plastic self-consistent (VPSC) [28,29], to the full-field crystal plasticity finite element (CPFE) [30–33] and Fast Fourier Transform-based (CP-FFT) [34] techniques, require a criterion for activating a slip system in order to predict slip activity. It is desirable that this criterion captures the rate sensitive motion of dislocations.

The strain rate and temperature sensitivity of the plastic deformation response of metals can in general be represented through the flow stress. The strain-rate sensitivity has been shown to be well represented by several constitutive models that are based on thermal activation kinetics developed by Kocks et al. [13]. One primary example is the mechanical threshold stress (MTS) model, which is due to the work of Follansbee and Kocks [35] and has been used in several applications involving dynamic deformation of materials [36,37], including an extension to crystal plasticity by assigning a MTS to each slip system [38]. In this