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Finite element implementation of dislocation-density-based crystal plasticity model and its application to pure aluminum crystalline materials

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ABSTRACT

A new time-integration algorithm is presented for a dislocation-density-based crystal plasticity model. This includes a monolithic iterative scheme in which stresses were solved simultaneously with dislocation densities based on the fully backward Euler method for the integration of the constitutive model. Furthermore, the heuristic convergence criterion based on the slip resistance, instead of dislocation densities, together with the stresses is employed to circumvent stability issues. A closed form of the consistent tangent moduli is also derived. The constitutive models and time-integration procedures have been implemented as a user-subroutine UMAT of a finite element program Abaqus. Representative comparisons between the numerical predictions and experimental data are then given to verify the robustness and stability of the current implementation of the dislocation-density-based crystal plasticity model. It is demonstrated that finite element calculations reproduce well the anisotropic hardening response of differently oriented pure aluminum single crystals under tension and the variation of pile-up patterns according to different initial crystallographic orientations during nanoindentation. Furthermore, the numerical procedure was used to predict the deformation response of the aluminum multicrystalline specimen under simple shear. Non-uniform deformation fields by the digital image correlation method and surface profiles by the shadow Moiré method were well reproduced by numerical predictions. In addition, the effect of the initial crystallographic orientation and the interaction effects among different crystals on the deformation response of the multicrystal are addressed.

1. Introduction

In recent years, many studies have been made to characterize the deformation response of polycrystalline materials, in particular when structural dimensions are approaching the microstructural length-scale of its constituent materials, i.e., from dozens of microns to the submicron range [1–8]. This is mainly due to the rapid growth of the electronics industry and accompanying development of microelectromechanical systems (MEMS) and nanoelectromechanical systems (NEMS) technologies. For examples, ductile crystalline materials commonly used for structural materials of electronics components consist of at most a few dozen grains or even several grains in their critical dimension (mainly thickness direction), e.g. metallic thin film electroplated on a Si substrate, solder bump, and intermetallic compounds formed at the interface between a bump and interconnects [9]. At this level, microstructural changes which affect the overall deformation response of polycrystalline aggregates mainly come from phenomena occurring at the single crystal level such as grain subdivision [10], the formation of micro-shear bands [11,12], lattice reorientation [7,13,14], and the formation of cell walls [15]. Furthermore, while the hardening rate of polycrystalline aggregates decreases continuously with plastic deformation, the deformation regime of single crystals can be divided into three stages according to its hardening rate [16]. In addition, the hardening response of single crystals depends significantly on the crystallographic orientation with respect to the sample axis, which manifests anisotropic behavior contrary to the polycrystalline materials with random texture. Thus, the demand for accurate and reliable numerical simulations that adequately capture the salient hardening behavior and microstructure evolution of single crystals is of prime importance to improve the predictive capability of the constitutive model and to gain further insight into the deformation mechanism of crystalline materials.

Since the pioneering work of Taylor [18], various constitutive models have been proposed to describe the anisotropic hardening behavior of single crystals in the literature. Two approaches are widely used [10]: the phenomenological model and physically based model.

The former mainly aims at predicting the overall stress–strain responses and texture evolutions of polycrystalline aggregates during

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forming processes where appropriate homogenization methods or finite element models [19–26] are employed to construct the average global responses from the anisotropic responses of individual grains. In many of these models, the slip resistance on a specific slip system is expressed as a function of accumulated crystallographic slips and the specific functional forms are adopted from classical hardening laws, e.g., the Voce-type saturation hardening law as discussed by Kalidindi and Anand [27] and Marin and Dawson [19], and the hyperbolic tangent law as described by Chang and Asaro [28]. Clearly, these phenomenological descriptions are computationally more efficient than the physically based model, which leads to the successful application of the crystal plasticity model to bulk forming processes such as rolling, forging, sheet forming, etc. However, in general, most of these phenomenological models fail in describing the salient features of the hardening behavior of single crystals [17]. Moreover, the increasing trend in the miniaturization of structural devices demands constitutive and numerical models to better describe the anisotropic response of single crystals. Motivated by these limitations, several researchers have proposed improved hardening models for the description of anisotropic behavior of single crystals during plastic deformation, e.g., Bassani and Wu [17], Weng [29] and Zhang et al. [30]. Since these hardening models are not related to any physical processes inducing plastic deformation, however, it is difficult to assign physical interpretations to the material parameters appearing in phenomenological models. Furthermore, as noted in Cuitino and Ortiz [31], the discrepancy in the form of the hardening interaction matrix between various models cannot be resolved when the assumption of constant latent hardening is applied. For example, in the work of Bassani and Wu [17], the diagonal terms which correspond to self-hardening are dominant over the off-diagonal terms describing the latent hardening effects, while in Peirce et al. [11] this is vice versa.

On the other hand, physically based crystal plasticity models attempt to characterize the deformation behavior of crystalline materials by taking the microstructural state of materials into account. This kind of model can directly track the evolution of microstructures during deformation and material parameters have their own physical interpretation; thus, it is expected to improve their predictive capability over the phenomenological model. In most works, dislocation densities are introduced as internal state variables to characterize the microstructure of materials and usually their evolution can be modeled based on the storage and annihilation processes for dislocations [32–34]. Earlier works on the development of hardening models employed single dislocation density to account for the microstructural state of materials. Tabourot et al. [34] established a framework for the development of the dislocation-density-based hardening model in which three kinetic equations are postulated to relate the crystallographic slip rate in an arbitrary slip system with the slip resistance and dislocation density. Cuitino and Ortiz [31] developed evolution equations governing dislocation motions from the statistical consideration of the forest dislocations in which the functional forms originally proposed by Gillis and Gilman [35] and Essmann and Rapp [36] were adopted. It predicts well the anisotropic hardening behaviors of Cu single crystals for various initial orientations and reveals that the discrepancies of hardening matrices in phenomenological models can be reconciled. Teodosiu et al. [32] proposed a dislocation-density-based hardening model including the interactions between different slip systems, which was employed for the simulation of inhomogeneously deformed crystalline aggregates at low homologous temperatures. It was shown that dislocations evolve towards some steady-state microstructures provided that a sufficient amount of monotonous deformation is allowed for along the same strain path. In the same way, Delaire et al. [37] applied the hardening model of Teodosiu et al. [32] to predict the deformation response of multicrystalline material during tensile deformation. In their work, full-field deformation fields in different crystallites of the multicrystal were compared with the simulation results. Harder [38] presented a dislocation-density-based hardening model incorporating back stress evolution and applied to the prediction of the Bauschinger effect. Recently, motivated by the experimental observation that the distribution of dislocations is very heterogeneous throughout the volume during plastic deformation, different approaches have been proposed to use two or three kinds of dislocation densities. The constitutive models in this category can be divided into various types depending on what kind of classification criterion are used to incorporate different dislocation densities into the framework of the single crystal plasticity model, e.g., types of dislocation, edge and screw [1,39–41]; mobility of dislocation, mobile and immobile [6]; and geometric character of dislocation, cell interior and cell walls [10,42]. More recently, Roters and co-workers have developed a hardening model based on the mobile and immobile dislocation in cell interiors and cell walls, respectively, which extend the work of Gottstein and co-workers [43,44]. Moreover, non-local models, including those that employ the lattice incompatibility tensor [4,5] or couple stress [45], have been developed to predict the well-known size effect in small-volume structures [46].

With the advancement of the constitutive models for crystal plasticity presented above, the crystal plasticity finite element model (CPFEM) has been applied to a number of deformation problems and has proved its predictive capability by comparing numerical results with experimental results [19,21–26]. Moreover, recently the grain-scale validation of the model has been carried out; the full-field deformation fields of the specimen during deformation were traced using non-contacting three-dimensional surface measurement techniques, e.g. digital image correlation (DIC) [13,2,37], and change of crystallographic orientations in each crystallites by electron backscatter diffraction (EBSD) [47,7]. These researches have been accomplished by the progresses in computer resources and the development of robust time-integration algorithms that allow for large-scale direct numerical simulations. However, the aforementioned success of the application of the crystal plasticity model is mainly based on the phenomenological hardening model which approximates the stress–strain response of single crystals as being hyperbolic since the incorporation of internal variables to the hardening model inevitably increases the complexity and computation time.

A comprehensive review of the time-integration algorithm of the rate-dependent single crystal plasticity model has been provided by Ling et al. [48]. In this study, the numerical scheme was classified into two main categories: a fully implicit algorithm based on the backward Euler method proposed by [1,4–6,19,20,27,31,49–51,55,56] and an explicit method proposed by [11,52–54], among others. Most notable in the framework of the implicit integration method is the work of Kalidindi and Anand [27] which presented a two-level iterative method for solving non-linear algebraic equations resulting from the discretization of the phenomenological slip-resistance-based hardening model. In the first level of the iterative scheme, the stresses are determined for a fixed state of the material and in a subsequent loop the kinetic variables, i.e. slip resistances are updated. These two loops are iteratively solved until convergence is achieved within specified tolerances. Several subsequent modifications for the two-level iterative method have been proposed to provide better numerical stability in such a way that the primary solution variable in the first loop has been replaced with the crystallographic shearing rate [31], elastic deformation gradient [55] or plastic deformation gradient [56], instead of the stress or an explicit method being applied in the second loop to accelerate the computing speed [55]. Most of the emphasis has been laid on the development of time-integration algorithms based on the rate-dependent crystal plasticity model but numerical algorithms for rate-independent models have also been developed. Interested readers can refer the work of Busso and Cailletaud [57] which presented a comprehensive investigation of the capabilities of the rate-dependent and rate-independent models for the prediction of complex multiaxial loading paths.

On the other hand, a few studies on the finite element implementa-