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Physically based crystal plasticity FEM including geometrically necessary dislocations: Numerical implementation and applications in micro-forming

Haiming Zhang [a,b,*], Xianghuai Dong [a]

[a] Institute of Forming Technology & Equipment, Shanghai Jiao Tong University, 1954 Hua Shan Road, Shanghai 200030, China
[b] Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

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ABSTRACT

Due to size effects, the conventional material constitutive models are no longer valid in the investigation of micro-forming processes. In this work, a nonlocal physically based crystal plasticity FEM is developed to investigate the size effects of micro-forming. Except for statistically stored dislocations, geometrically necessary dislocations on the slip systems are introduced and calculated via the mesh-free paradigm. The micro-tensile and micro-deep drawing experiments of polycrystalline copper foils with different thicknesses and grain sizes are used to calibrate the presented nonlocal model. The comparison between simulations and experiments shows that the nonlocal physically based crystal plasticity FEM is capable of describing both the first order and the second order size effects of the micro-forming processes, and providing more microstructural clues for the interpretation of these size effects. Furthermore, the simulations of micro-deep drawings demonstrate that the presented nonlocal method is robust in the simulations with complex contact boundary conditions.

1. Introduction

The rapid development of micro-electro-mechanical system and micro system technology places a greater demand on the mass fabrication of micro-parts. Micro-forming, which manufactures micro-parts with the desirable geometries via plastic deformation, is attractive for the low-cost and mass production of micro-parts [1,2]. Lots of micro-forming processes have been extensively explored in recent years, such as upsetting, extrusion, bending, deep drawing, and blanking [3–6]. As the size of micro-parts is scaled down to the micron level, which is close to the intrinsic microstructural length scale of materials, *e.g.*, the grain size and the mean free path of dislocations, size effects occur obviously. It is found that the well-established knowledge of the conventional metal forming processes is not applicable in micro-forming processes due to the size effects. The trial-and-error approach is generally used for the design of micro-forming processes. However, such method is time-consuming and costly, and the quality of parts is not assured [7]. The optimization of micro-forming needs more comprehensive understanding of the mechanical behaviors of materials. Due to the lack of intrinsic material length scale and microstructural information, the traditional material models are not yet sufficient to describe the mechanical behaviors (*i.e.*, various size effects) of materials at micro-scale. Therefore, developing the state-of-art models and numerical techniques are crucial for the investigation and optimization of micro-forming processes.

The size effects at micro-scale are often divided into two categories, *i.e.*, the first order and the second order size effects [8,9]. The first order size effects include all effects resulting from the discrete granular anisotropic nature of microstructures. For example, the plastic deformation behavior is dominated by a few grains located in the deformation region, the material microstructures are not homogeneous, the grain size, crystallographic orientation, and dislocation density show more pronounced effects on the mechanical behaviors of metallic polycrystalline materials at micro-scale. The second order size effects mainly refer to the strengthening effect of strain gradients or slip gradients due to the inhomogeneous plastic deformation.

For polycrystalline metals at micro-scale, because of limited grains in the deformation region, the first order size effects involve the influence of the grain size (D), sample size (*e.g.*, thickness t), orientation, *etc.* Janssen et al. conducted the uniaxial tensile experiments of pure aluminum foils with a few grains across the thickness, and found that the ratio $t/D(\lambda)$ has a marked impact

* Corresponding author at: Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany.
E-mail address: hmzhang10@gmail.com (H. Zhang).

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on flow stress, it also shows that the classic Hall–Petch relation is not suitable for this case [10]. Lederer et al. performed the tensile tests of high purity aluminum foils with different thicknesses at different temperatures. It is found that t and D are the major contributions to the size effects [11]. The micro-tensile tests of nickel polycrystals show that λ also affects the hardening stages, flow stress, intragranular and intergranular back stress of samples [12]. Kals and Eckstein found from the tensile experiments of pure copper foils that the grains in the surfaces weaken the global strength of samples, it is explained that theses grains have more active slip systems due to less constraint [13]. Liu et al. performed the micro-bending experiments of pure copper foils, and found that the elastic anisotropy of surface grains due to the difference of the crystallographic orientation is the main reason for the scatter of springback angles [14].

The strain gradient strengthening effect in the micro-scale plastic deformation has received considerable attentions during the past two decades. Experimental researches have been carried out for different materials and deformation modes, such as micro-torsion [15], micro-bending [16], and micro-indentation [17,18]. All these experiments support that the strain gradients strengthen materials. There is a general agreement that the strain gradient effect, which usually manifests itself at micro-scale, can be attributed to hardening enabled by geometrically necessary dislocations (GNDs) [19]. GNDs represent an extra storage of dislocations required to accommodate the lattice curvature which arises whenever there is inhomogeneous plastic deformation [20]. In contrast, statistically stored dislocations (SSDs) evolve from the random trapping processes of dislocations during plastic deformation, which do not give rise to significant lattice curvature. Recent years, high-resolution electron backscattered diffraction (HR-EBSD) has become an emerging tool to characterize GNDs densities by analysis of lattice curvature [21,22]. However, in situ distribution of GNDs during plastic deformation and quantitative determination of full-field GNDs are currently not available.

Obviously, the plastic deformation of polycrystalline metals at micro-scale generally involves both the first order and the second order size effects, a detailed study of microstructure evolution and deformation mechanism must be conducted to investigate these size effects. Though the continuum surface layer models [2,5,23] are capable of describing several first order size effects, they fail to describe the second order size effects. While the continuum strain gradient plasticity models [15,24,25] are able to describe the strain gradient effect, they cannot analysis the first order size effects which are intrinsically present in engineering problems. Moreover, the continuum material models ignore the crystallographic orientation and the discreteness (*i.e.,* the granular nature) of microstructures. Recently, the widely used micro-mechanical models, *i.e.,* crystal plasticity (CP) models, which describe the first order size effects well, were elaborated into nonlocal CP models to consider the second order size effects simultaneously [26–33]. The length scale dependent internal state variables (ISVs), *e.g.,* slip gradients or GNDs densities of the slip systems are introduced into the constitutive models. Among various nonlocal CP models, nonlocal dislocation density based crystal plasticity finite element method (CPFEM) [28–33], which utilizes the densities of SSDs and GNDs as ISVs, and use the FEM framework to deal with boundary conditions, is a promising tool to probe the size effects of the micro-scale plastic deformation.

However, the numerical implementation of the nonlocal dislocation density based CP models into the FEM framework raises a number of fundamental problems. The evolution law of GNDs densities contains the gradients of shear rate of each slip system, *i.e.,* the GNDs densities in the considered integration point (IP) depend on not only its plastic deformation state, but also the plastic deformation state of its surrounding IPs. The nonlocal characteristic of GNDs densities makes it cannot be obtained directly from the classic FEM framework. Meissonnier et al. implemented a nonlocal model via writing a mix integration user element, the displacement field is represented by a standard quadratic 20-nodes iso-parametric element with reduced $(2 \times 2 \times 2)$ integration, while the slip rate gradients are interpolated by a linear shape functions associated with the eight corner nodes and full $(2 \times 2 \times 2)$ integration [34]. Dunne et al. adopted a similar scheme for the plane strain deformation [35]. Evers et al. [28] and Arsenlis et al. [29] treated the densities of GNDs and SSDs as additional degrees of freedom for every node, derived a set of discretized iterative equations which were implemented in in-house FEM codes based on a standard Galerkin approach. Such scheme does not require high order elements, can be solved by using C^0-continuous elements. However, it relies on the additional dislocation density flux boundary conditions, which are difficult to formulate for the complicated boundary value problems. Ma et al. [30], Lee and Chen [36] implemented nonlocal CP models into commercial FEM codes via writing an user material subroutine (UMAT) rather than an user element subroutine. The procedure of their methods is: after the slip rates and plastic deformation gradients at the eight IPs have been fully collected, these variables at the eight nodes are obtained by an extrapolation scheme, then the strain gradients and GNDs densities at the IPs are determined by calculating the spatial derivatives of the linear shape functions. Such scheme can be achieved in the updating of material constitutive models, so it makes the nonlocal CPFEM usable in the simulation of complex contact problems, *e.g.,* micro/nano-indentation [36,37]. However, due to the extrapolation scheme from the IPs to the nodes, this scheme is limited to the specific type of elements, *e.g.,* the full-integration element.

The aim of this paper is to formulate a new numerical implementation of the nonlocal physically based material model without modification and restriction of the conventional FEM codes, which makes the nonlocal CPFEM comparatively robust and attractive to be used in the simulations with complex boundary conditions, *e.g.,* micro-forming. The mesh-free methodology is adopted to re-construct the shape functions of nonlocal variables, *i.e.,* the GNDs densities of the considered IP are evaluated according to its neighboring IPs in a local compact domain. The implementation of presented nonlocal model is the same as a local one, the calculation of nonlocal variables is achieved in the updating of material constitutive model. The presented model is implemented into ABAQUS/Explicit by writing an user material subroutine VUMAT to investigate the first order and the second order size effects of micro-forming, and its performance is verified by the comparison with experiments of micro-tension and micro-deep drawing.

2. Theory

2.1. Finite deformation crystal plasticity theory

In this work, the kinematics of crystal plasticity model is established in the hyperelastic frame. The multiplicative decomposition of the total deformation gradient $\mathbf{F}$ can be expressed as [38]

$$\mathbf{F} = \mathbf{F}^{e}\mathbf{F}^{p} \tag{1}$$

where $\mathbf{F}^{p} = \partial\overline{\mathbf{X}}/\partial\mathbf{X}$ and $\mathbf{F}^{e} = \partial\mathbf{x}/\partial\overline{\mathbf{X}}$. $\mathbf{F}^{p}$ accounts for the inelastic shear deformation along the crystalline slip planes, maps the initial configuration ($\mathbf{X}$) into the stress-free intermediate configuration ($\overline{\mathbf{X}}$). $\mathbf{F}^{e}$ is in charge of the rotation and elastic distortion of the lattice, and maps the intermediate configuration into the current configuration ($\mathbf{x}$). By the time differentiation of Eq. (1), the additive decomposition of the velocity gradient can be obtained as

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{F}}^{e}\mathbf{F}^{e\text{-}1} + \mathbf{F}^{e}\mathbf{L}_{0}^{p}\mathbf{F}^{e\text{-}1} \tag{2}$$