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Research paper

Size-dependent crystal plasticity: From micro-pillar compression to bending

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ABSTRACT

Size-dependent crystal plasticity of metal single crystals is investigated using finite-element method based on a phenomenological crystal-plasticity model, incorporating both first-order and second-order effects. The first-order effect is independent of the nature of the loading state, and described by three phenomenological relationships based on experimental results. The second-order effect is considered in terms of storage of geometrically necessary dislocations, affected significantly by the loading state. The modelling approach is shown to capture the influence of loading conditions on the sample size effect observed in compression and bending experiments. A modelling study demonstrates the subtleness and importance of accounting for first-order and second-order effects in modelling crystalline materials in small length-scales.

1. Introduction

It is well known that metallic single crystals at the micron and submicron scale exhibit different mechanical behaviour in comparison to its bulk counterpart. In almost all experimental studies, the phenomenon of ‘smaller is stronger’ has been observed (see e.g. Greer and De Hosson, 2011). From a classical standpoint, the sample size effect is typically described by a power-law relationship (similar to the Hall-Petch effect), $\sigma_f = \sigma_0 + Kd^{-n}$ or $\sigma_f = Kd^{-n}$, where σ_f is the measured flow stress, d is the characteristic sample size, and σ_0, K and n are experimentally fitting parameters (Hug et al., 2015). For different single crystals, experimental results obtained by micro-pillar compression show that n is typically in the range of 0.6–1.0 for FCC metals and 0.5 or less for BCC metals (Tarleton et al., 2015). Experimental data for HCP metals indicate that n is ~0.5 for prismatic slip in Ti (Sun et al., 2011), 0.8 (Ye et al., 2011) or 0.4 (Byer and Ramesh, 2013) for basal slip and 0.2 for pyramidal slip in Mg (Byer and Ramesh, 2013). Apart from the size-dependent strengthening effect, a size-dependent softening was also reported when a reverse loading was applied on the cantilever-beam of single-crystal copper (Demir and Raabe, 2010).

Although the sample size effect of single crystal is experimentally described by the power-law relationship, the underlying physical mechanism driving size effects is still debated. Geers et al. (2006) categorized the size effect in polycrystalline metals into (i) intrinsically first-order effect, which was considered to cover all effects resulting from the nature of microstructure and (ii) second-order effect,[1] which was considered to result from gradients of deformation (strain gradient, slip gradient, etc.). We adopt a similar classification in this paper for single-crystal metals. In a single-crystal sample, as there is no microstructural feature related to grain boundary and the heterogeneity of grains, the first-order effect can be determined from several dislocation-mediated mechanisms, including source-limitation, dislocation starvation and source-truncation hardening mechanisms, amongst others (El-Awady, 2015; Kiener et al., 2006). The second-order effect mainly originates from inhomogeneous plastic deformation or slip gradient in a single-crystal sample (e.g. due to bending).

Due to the different underlying physical mechanisms, a quantitative difference may be observed for the sample size effect measured in different loading conditions. For example, when the power-law relationship is employed to characterize the sample size effect in a Cu single crystal, the measured n is about 0.4 for micro-pillar compression (Kiener et al., 2006) and 0.8 for cantilever beam experiments (Motz et al., 2005). In Ti, the value of K for prismatic slip is about 131 Pa-m from micro-pillar compression tests (Sun et al., 2011) but 354 Pa-m from cantilever-beam experiments (Gong and Wilkinson, 2011), although the values of σ_0 and n are comparable for the two loading conditions. These experimental data indicates that the sample size effect in bending, due to the

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[1] Not to be confused with higher order (gradient) theories.

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coexistence of first-order and second-order effects (i.e. externally imposed stress/strain gradients), is more pronounced than that in uniaxial compression where first-order effect dominate. Here, the dependence of size effect on loading conditions cannot be depicted by the popular power-law relationship. Moreover, the experimental results of Maass et al. (2009) indicate that the power-law relationship based on flow stress could overestimate the true size effect due to the influences of boundary constraints on the measured hardening behaviour. Consequently, the simplified power-law relationship is incomplete (or incorrect) in describing size effect, especially when both first-order and second-order effects dominate.

To overcome the drawback of the power-law relationship approach, crystal-plasticity (CP) modelling was employed to help extract the nature of size effect in single-crystal metal (Gong and Wilkinson, 2011; Raabe et al., 2007). From a modelling perspective, the first-order effect is typically modelled using conventional CP based constitutive models, which suffer from several short comings. The second-order effect may be described by strain-gradient-based model (Geers et al., 2006). In a CP modelling framework, the second-order effect was general modelled as plastic strain gradient (Roters et al., 2010). The non-uniform plastic deformation was generally associated with the storage of geometrically necessary dislocations (GNDs) in contrast to statistically stored dislocations (SSDs) that is considered independent of plastic strain gradient (Faghihi and Voyiadjis, 2012). Size-dependent work-hardening will become significant when the storage of GNDs is comparable to SSDs, leading to the second-order effect. Such a strain-gradient effect, associated with GNDs, has been introduced into CP model by two approaches. One is based on high-order CP theory that requires additional boundary conditions which are difficult to determine physically (Reuber et al., 2014). The other being a lower-order strain-gradient CP theory, where the storage of GNDs are introduced into the evolution of SSDs and calculation of slip-system resistance (Ma et al., 2006).

Our primary goal is to characterize both the first-order and second-order effects in small-scale single crystals using a CP theory. Three phenomenological relationships are proposed to describe the first-order effect based on micro-pillar compression experiments and discrete dislocation dynamics (DDD) simulation studies. A low-order strain-gradient CP approach is adopted to introduce the second-order effect in the current study. Contributions of the second-order effect, in addition to the first-order one, are estimated from cantilever-beam experimental data. Numerical studies show that the proposed modelling framework is capable to characterise size effects under macroscopically homogeneous and in-homogeneous loading states.

The paper is organized as follows: in Section 2, a self-contained description of the governing relations of proposed size-dependent CP model is presented. Section 3 comprises a finite-element modelling strategy implemented in a general commercial finite element software package ABAQUS. In Section 4, results of the implementation are presented and discussed. The paper ends with some concluding remarks in Section 5.

2. Constitutive description of first-order and second-order effects

In this section, a phenomenological size-dependent crystal plasticity (SDCP) model is proposed, which accounts for the first-order and second-order effects of crystalline metals. Standard notations are adopted here: scalars are in italics, vectors and tensors are represented with lower-case and upper-case bold letters.

First, for completeness, the classical CP theory adopted in this study is reviewed. Deformation gradient $\mathbf{F}$, can be decomposed into the elastic and plastic parts (Roters et al., 2010), as,

$$\mathbf{F} = \mathbf{F_e F_p}, \tag{1}$$

where the subscripts 'e' and 'p' denote the elastic and plastic parameters, respectively. The multiplicative decomposition is non-unique. By applying the product rule of differentiation, one can obtain the rate of the total deformation gradient $\dot{\mathbf{F}}$:

$$\dot{\mathbf{F}} = \dot{\mathbf{F}}_\mathbf{e}\mathbf{F_p} + \mathbf{F_e}\dot{\mathbf{F}}_\mathbf{p}. \tag{2}$$

Therefore, the velocity gradient $\mathbf{L}$ can be introduced following its definition $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$, as,

$$\mathbf{L} = \dot{\mathbf{F}}_\mathbf{e}\mathbf{F}_\mathbf{e}^{-1} + \mathbf{F_e}(\dot{\mathbf{F}}_\mathbf{p}\mathbf{F}_\mathbf{p}^{-1})\mathbf{F}_\mathbf{e}^{-1} = \mathbf{L_e} + \mathbf{L_p}. \tag{3}$$

It is assumed that the plastic velocity gradient, $\mathbf{L_p}$, is induced by shearing on each slip system. Hence, $\mathbf{L_p}$ is formulated as the sum of the shear rates on all slip systems, i.e.

$$\mathbf{L_p} = \sum_{\alpha=1}^{N} \dot{\gamma}^{(\alpha)} \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}, \tag{4}$$

where, $\dot{\gamma}^{(\alpha)}$ is the shear slip rate on the slip system α, N is the total number of slip systems, and unit vectors $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ define the slip direction and the normal to the slip plane in the deformed configuration, respectively. Furthermore, the velocity gradient can be expressed in terms of a symmetric rate of stretching $\mathbf{D}$ and an antisymmetric rate of spin $\mathbf{W}$, as,

$$\mathbf{L} = \mathbf{D} + \mathbf{W} = (\mathbf{D_e} + \mathbf{W_e}) + (\mathbf{D_p} + \mathbf{W_p}). \tag{5}$$

Using Eqs. (3) and (4), it can be deduced

$$\mathbf{D_e} + \mathbf{W_e} = \dot{\mathbf{F}}_\mathbf{e}\mathbf{F}_\mathbf{e}^{-1}, \mathbf{D_p} + \mathbf{W_p} = \sum_{\alpha=1}^{N} \dot{\gamma}^{(\alpha)} \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}. \tag{6}$$

Following the work of Huang (1991), the constitutive law is expressed as the relationship between the elastic part of the symmetric rate of stretching, $\mathbf{D_e}$, and the Jaumann rate of Cauchy stress, $\overset{\nabla}{\boldsymbol{\sigma}}$, i.e.

$$\overset{\nabla}{\boldsymbol{\sigma}} + \sigma(I : \mathbf{D_e}) = \mathbf{C} : (\mathbf{D} - \mathbf{D_p}), \tag{7}$$

where, $\mathbf{I}$ is the second-order unit tensor, $\mathbf{C}$ is the fourth order, possibly anisotropic, elastic stiffness tensor. The Jaumann stress rate is expressed as

$$\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\sigma} - \mathbf{W_e}\boldsymbol{\sigma} + \sigma\mathbf{W_e}. \tag{8}$$

On each slip system, the resolved shear stress, $\tau^{(\alpha)}$, is expressed by Schmid law,

$$\tau^{(\alpha)} = (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}) : \boldsymbol{\sigma}. \tag{9}$$

The relationship between the shear rate, $\dot{\gamma}^{(\alpha)}$, and the resolved shear stress, $\tau^{(\alpha)}$, on the slip system, α, is expressed by the power law proposed by Hutchinson (1976):

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^n \mathrm{sgn}(\tau^{(\alpha)}) \tag{10}$$

where, $\dot{\gamma}_0$ is the reference shear rate, $g^{(\alpha)}$ is the slip resistance and n is the rate sensitivity parameter. Next, the model is developed to account for the first-order and second-order effects, which are introduced into the calculation of $g^{(\alpha)}$.

2.1. First-order effect

In the absence of strain gradient, it is generally accepted that $g^{(\alpha)}$ is determined by the content of statistically stored dislocations (SSDs) in the component. For a single crystal at macro-scale, nucleation of dislocations is relatively easy (El-Awady, 2015) due to the geographic abundance of nucleation sites. Thus, slip resistance in the macro-scale can be described by the empirical Taylor model (El-Awady, 2015). However, at smaller length scales,