

Dislocation-based constitutive model of crystal plasticity for the size effect of single crystalline micropillar samples

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Received 29 October 2015

Abstract

In this study, based on the Orowan equation and the principle of Bergstrom dislocation evolution, the plastic mechanical response of single crystalline micropillars is investigated by considering dislocation evolution. According to the single-arm source model, a physically revised Peirce–Asaro–Needleman (PAN) hardening model is proposed that can describe size-dependent hardening flow. The dislocation evolution parameters greatly affect the size-dependent plastic behavior of the single crystalline micropillars. Linking to the crystal plasticity finite element (CPFE) method, a physical plastic constitutive model with the framework of the CPFE method is proposed to solve the size-dependent boundary value problem. Compared with the results based on the original PAN hardening model, the proposed constitutive model can provide mechanical responses in different sizes, depending on the shear strain in each slip plane. If the non-friction condition between the rigid punch and the top surface of the pillar under uniaxial compression is considered, the results show that the shear band of the pillar mainly results from shear deformation on the slip plane with the maximum Schmid factor. Otherwise, the actual shear band deformation of the micropillars is complicated and combined with the other slip planes, that is, a multislip system. The results also indicate that friction affects size-dependent hardening.

Key words : Bergstrom dislocation evolution, Orowan equation, Size effect, Constitutive equation, Elastic-plastic deformation

1. Introduction

Constitutive laws, kinematics, homogenization, physical analyses, and multiscale calculations in crystal plasticity finite-element (CPFE) modeling are widely used to describe elastic–plastic deformation of anisotropic heterogeneous crystalline matter (Bechker, 1998; Evers et al., 2004; Gerken and Dawson, 2008; Gurtin et al., 2000; Raabe and Becher, 2000; Roters et al., 2005). The CPFE model can describe both shape changes (symmetric part) and lattice rotations (skew-symmetric part) (Peirce et al., 1982; Gerken and Dawson, 2008). The CPFE model might be improved by using the extensive knowledge gained from experimental and theoretical studies of single crystalline deformation and introducing the further development of continuum field theories (Evers et al., 2004; Gurtin et al., 2000). Therefore, the CPFE method can be used to investigate the size-dependent plastic behavior of single crystalline micropillars (SCMs) by considering the lattice deformation and the crystallographic system.

In terms of the plasticity of SCMs, the size-dependent mechanical response (size effect), including extremely high strength and unsmooth hardening (Dimiduk et al., 2005; Uchic et al., 2004), should be considered. There are some micromechanisms of size-dependent yield strength of the SCMs, which are commonly based on the inner defects, such as source truncation (Kiener et al., 2009), dislocation starvation (Shan et al., 2008), source starvation and inner dislocation pile-up (Parthasarathy et al., 2007; Pan et al., 2015). According to these considerations, prediction of the yield strength for the SCMs has been studied and these theories, such as the single-arm source (SAS) model, are different from conventional scale-free solid mechanics (Pan et al., 2015; Parthasarathy et al., 2007). The CPFE method has also been used to describe the anomalous hardening by adding experimental data, such as the recent studies of displacement burst (Zhang and Shang, 2014; Zhang et al., 2012, 2014) and dislocation starvation (Gao et al., 2010).

However, the hardening model and constitutive laws used in these studies did not involve any physical size-dependent considerations. The reason for the size-dependent plastic flow is still unclear, and the physical mechanism of this phenomenon is also not well understood. Moreover, the physical hardening model can affect the constitutive law because of the mechanical effect on dislocation motion. Therefore, it is necessary to build the CPFE framework by combining the physical model of the yield stress and the dislocation-based hardening model to obtain the constitutive law with the size effect.

The objective of this work is to develop a constitutive model with the CPFE framework that accounts for dislocation physics to describe the size-dependent deformation. The relationship between the dislocation density and the plastic strain is derived based on the Orowan equation and the principle of Bergstrom dislocation evolution, and the physical model of yield stress is provided from the SAS model. We then redefine the original Peirce, Asaro, and Needleman (PAN) hardening model by considering the effective dislocation length and dislocation evolution. Finally, the yield stresses and redefined PAN model are included in the CPFE model. The dislocation evolution parameters are determined by fitting to the experimental data, and they are used to describe the size-dependent characteristics of plastic flow. Comparing with results based on the original PAN hardening model, the proposed model can describe size-dependent mechanical responses. Further discussion about the friction effect between the punch and the top surface of the pillar under uniaxial compression is given based on the stress-strain response and shear band deformation inside the pillar.

2. Dislocation-based model for the size effect

2.1 Relationship between plastic strain and dislocation density under uniaxial compression

The total dislocation density can be expressed as

$$\rho_{\text{total}} = \rho_{\text{mobile}} + \rho_{\text{trapped}}, \quad (1)$$

where ρ_{total} is the total dislocation, ρ_{mobile} is the mobile dislocation and ρ_{trapped} is the trapped dislocation. The rate of plastic shear strain $\dot{\gamma}_p$ in any slip system can be expressed according to the Orowan equation as

$$\dot{\gamma}_p = \rho_{\text{mobile}} b \bar{v}, \quad (2)$$

where $\bar{v}$ is the average velocity of dislocations and b is the Burgers vector. Assuming that the mobile dislocation density is not dependent to time because of the dislocation movement in a short time, Eq. (2) can be integrated simply according to time. By averaging the quantities for the whole single crystalline pillar with one or a few active slip systems, Eq. (2) is reformulated using the uniaxial plastic compressive strain ε_p of the whole single crystalline pillar and the average total length of mobile dislocation $\bar{L}_m$ as follows.

$$\varepsilon_p = \rho_{\text{mobile}} b \bar{L}_m. \quad (3)$$

$\bar{L}_m$ can be expressed by the average length of the mobile dislocation and the number of mobile dislocation as (Hill and Rice, 1972)

$$\bar{L}_m = n \bar{d}_m = n / \sqrt{\rho_{\text{mobile}}}, \quad (4)$$

where n is the number of mobile dislocations and $\bar{d}_m$ is the average length of the mobile dislocations. n is related to the sample dimensions and initial dislocation density for the case of micro-sized pillars (Parthasarathy et al., 2007):

$$n = \text{Integer} \left[\frac{\rho_0 \pi R^2}{s} \right], \quad (5)$$

where R is the radius of the pillar specimen, and s is the number of slip systems. In this paper, the parameters are selected to be $s = 12$ for face-centered cubic (fcc) crystals. In this case, by substituting Eq. (4) into Eq. (3), the following equation can be obtained:

$$\rho_{\text{mobile}} = (\varepsilon_p / bn)^2. \quad (6)$$

According to the principle of Bergstrom dislocation evolution (Hill and Rice, 1972), the trapped dislocation density can be expressed as

$$\rho_{\text{trapped}} = \frac{1}{\Omega^2} \left\{ k^* - \frac{k^* - \Omega \sqrt{\rho_0}}{\exp(\Omega \varepsilon_p / 2)} \right\}^2, \quad (7)$$

where ρ_0 is the initial dislocation density, and k^* and Ω are the parameters of dislocation evolution on the increase of trapped dislocation and the dislocation annihilation, respectively. We assume that the initial dislocation is only the initial trapped dislocation, because there are very few initial mobile dislocations for the micropillars (Gao et al., 2010; Parthasarathy et al., 2007).

Therefore, the total dislocation density can be obtained by substituting Eqs. (6) and (7) into Eq. (1):

$$\rho_{\text{total}} = \rho_{\text{mobile}} + \rho_{\text{trapped}} = (\varepsilon_p / bn)^2 + \frac{1}{\Omega^2} \left\{ k^* - \frac{k^* - \Omega \sqrt{\rho_0}}{\exp(\Omega \varepsilon_p / 2)} \right\}^2. \quad (8)$$

The dislocation evolution parameters (k^* and Ω) are determined from the experimental data, which will be introduced in Section 2.3.

2.2 Initial yield stress and constitutive equation of the extended SAS model

According to the theory of dislocation starvation and exhaustion, the statistical behavior of dislocations is used to describe the strength (Bei et al., 2008; Pan et al., 2015; Parthasarathy et al., 2007; Schneider et al., 2013; Shan et al., 2008). Based on this view, the SAS model derived from statistical mechanics can be used to describe the size-dependent strength of SCMs (Parthasarathy et al., 2007).

The critical resolved shear stress (CRSS) of micropillars is related to the effective dislocation source length λ . Thus, it can be expressed as the SAS model (Parthasarathy et al., 2007):

$$\tau_{\text{SAS}}^0 = \tau_0 + 0.5\mu b \sqrt{\rho_0} + \frac{\alpha\mu b}{\bar{\lambda}_{\text{max}}}, \quad (9)$$

where μ is the shear modulus, τ_0 is the Peierls–Nabarro stress, α is the constant and $\bar{\lambda}_{\text{max}}$ is the effective average longest length of the dislocation sources (remind that $\bar{\lambda}_{\text{max}}$ is dependent to the radius of pillar, as written in ref. of Pan et al., 2015). Equation (9) is used to describe the initial yield stress accounting for the initial dislocation density ρ_0 .

If the subsequent plastic process is represented, the SAS model can be extended to express the function of the dislocation density ρ and the plastic strain ε_p instead. In this case, Eq. (8) should be used to describe the evolution of dislocations in the micropillars according to the plastic strain. Therefore, substituting Eq. (8) into Eq. (9), the shear stress on the slip plane is

$$\tau_{\text{SAS}}^f = \tau_0 + 0.5\mu b \left[(\varepsilon_p / bn)^2 + \frac{1}{\Omega^2} \left\{ k^* - \frac{k^* - \Omega \sqrt{\rho_0}}{\exp(\Omega \varepsilon_p / 2)} \right\}^2 \right]^{0.5} + \frac{\alpha\mu b}{\bar{\lambda}_{\text{max}}}, \quad (10)$$

where $\bar{\lambda}_{\text{max}}$ can be simulated using the statistics method (Parthasarathy et al., 2007).

The τ_{SAS}^0 and τ_{SAS}^f values are used to describe the CRSS and the subsequent yield shear stress of the micropillars, respectively. The τ_{SAS}^0 in Eq. (9) agrees well with experimental data (Parthasarathy et al., 2007). However, the values of the parameters k^* and Ω in Eq. (10) are still unknown. In the following, the values of these parameters will be determined by fitting to the experimental data.

2.3 Determination of k^* and Ω

By substituting Eq. (10) into the equation $\sigma = M_\sigma \tau_{\text{SAS}}^f$ under uniaxial compression, where M_σ is the Taylor-like factor which phenomenologically links the local shear stress to the global uniaxial stress (Beyerlein and Tomé, 2008; Hirth and Lothe, 1982), the hardening ratio θ can be expressed by differentiation as

$$\theta = \frac{d\sigma}{d\varepsilon_p} = \frac{M_\sigma \mu b}{4\sqrt{\rho_{\text{total}}}} \frac{2}{nb} (\varepsilon_p / nb) + \frac{M_\sigma \mu b}{4\sqrt{\rho_{\text{total}}}} (k^* \sqrt{\rho_{\text{trapped}}} - \Omega \rho_{\text{trapped}}) = \theta^m + \theta^t. \quad (11)$$

θ^m and θ^t are the hardening rate affected by mobile dislocations and the hardening rate affected by trapped dislocations, respectively. That is,

$$\theta^m = \frac{M_\sigma \mu b}{4\sqrt{\rho_{\text{total}}}} \frac{2}{nb} (\varepsilon_p / nb). \quad (12)$$

When $\varepsilon_p = 0$, θ_y is the hardening rate at the initial yielding, which can be obtained as $\theta_y = \theta (\varepsilon_p = 0)$. Thus,

$$\theta_y = \frac{M_\sigma \mu b}{4} (k^* - \Omega \sqrt{\rho_0}). \quad (13)$$

Differentiating Eq. (7) with respect to plastic strain ε_p , it gives

$$\frac{d\rho_{\text{trapped}}}{d\varepsilon_p} = k^* \sqrt{\rho_{\text{trapped}}} - \Omega \rho_{\text{trapped}}. \quad (14)$$

Integrating Eq. (14), the relationship between the plastic strain and the trapped dislocation density is

$$\varepsilon_p = \frac{2}{\Omega} \ln \left(\frac{k^* - \Omega \sqrt{\rho_0}}{k^* - \Omega \sqrt{\rho_{\text{trapped}}}} \right) = \frac{2}{\Omega} \ln \left(\frac{\sqrt{\rho_{\text{trapped}}} \theta_y}{\sqrt{\rho_{\text{total}}} \theta^t} \right), \quad (15)$$

where

$$\theta^t = \frac{\sqrt{\rho_{\text{trapped}}}}{\sqrt{\rho_{\text{total}}}} \theta_y \exp\left(-\frac{\Omega \varepsilon_p}{2}\right). \quad (16)$$

The stress σ can be obtained by substituting Eqs. (16) and (12) into Eq. (11) and then integrating:

$$\sigma - \sigma_0 = \frac{2\theta_y}{\Omega} \frac{\sqrt{\rho_{\text{trapped}}}}{\sqrt{\rho_{\text{total}}}} [1 - \exp(-\frac{\Omega \varepsilon_p}{2})] + \frac{M_\sigma \mu b}{4\sqrt{\rho_{\text{total}}}} (\varepsilon_p / nb)^2, \quad (17)$$

where σ_0 is the experimental initial yield stress. Equations (8), (11), and (17) can be used to obtain the dislocation evolution parameters (k^* and Ω) by fitting to the experimental data with the least-squares method.

The fitted results are shown in Figs. 1 and 2. In Fig. 1, Eq. (17) was used to fit the Ni experiment data (Dimiduk et al., 2005; Kiener et al., 2009) with the least-squares method, and the determined parameters are given in Table 1. In Fig. 2, the same method was used to obtain the parameters of Cu by comparing with the experiments for the pillars with diameter $d \sim 1 \mu\text{m}$ and $d \sim 4 \mu\text{m}$ (Hirouchi and Shibutani, 2014), and the results are also given in Table 1. In Figs. 1(a) and (b), the hardening flows for $d \sim 10 \mu\text{m}$ and $\sim 20 \mu\text{m}$ involving a series of small strain bursts are close to that of the bulk material (Dimiduk et al., 2005). In Fig. 1(c), the hardening flow for $d \sim 5 \mu\text{m}$ specimens includes obvious strain bursts, and the hardening process shows different evolution of dislocations from the bulk material, which is the size

effect of hardening flow (Dimiduk et al., 2005). In Fig. 2, the hardening flow for $d \sim 1 \mu\text{m}$ is more than twice as strong as that for $d \sim 4 \mu\text{m}$. In Table 1, the k^* and Ω values for $d \sim 10$ and $\sim 20 \mu\text{m}$ in Ni are nearly the same. Meanwhile, the k^* value for $d \sim 5 \mu\text{m}$ in Ni is larger than that for $d \sim 10 \mu\text{m}$, and the Ω value for $d \sim 5 \mu\text{m}$ in Ni is smaller than that for $d \sim 10 \mu\text{m}$. The same conclusion can be obtained by comparing the data of Cu in Table 1. That is, the material of the smaller micropillars has a larger k^* value and a smaller Ω value, which suggests more active dislocation evolution.

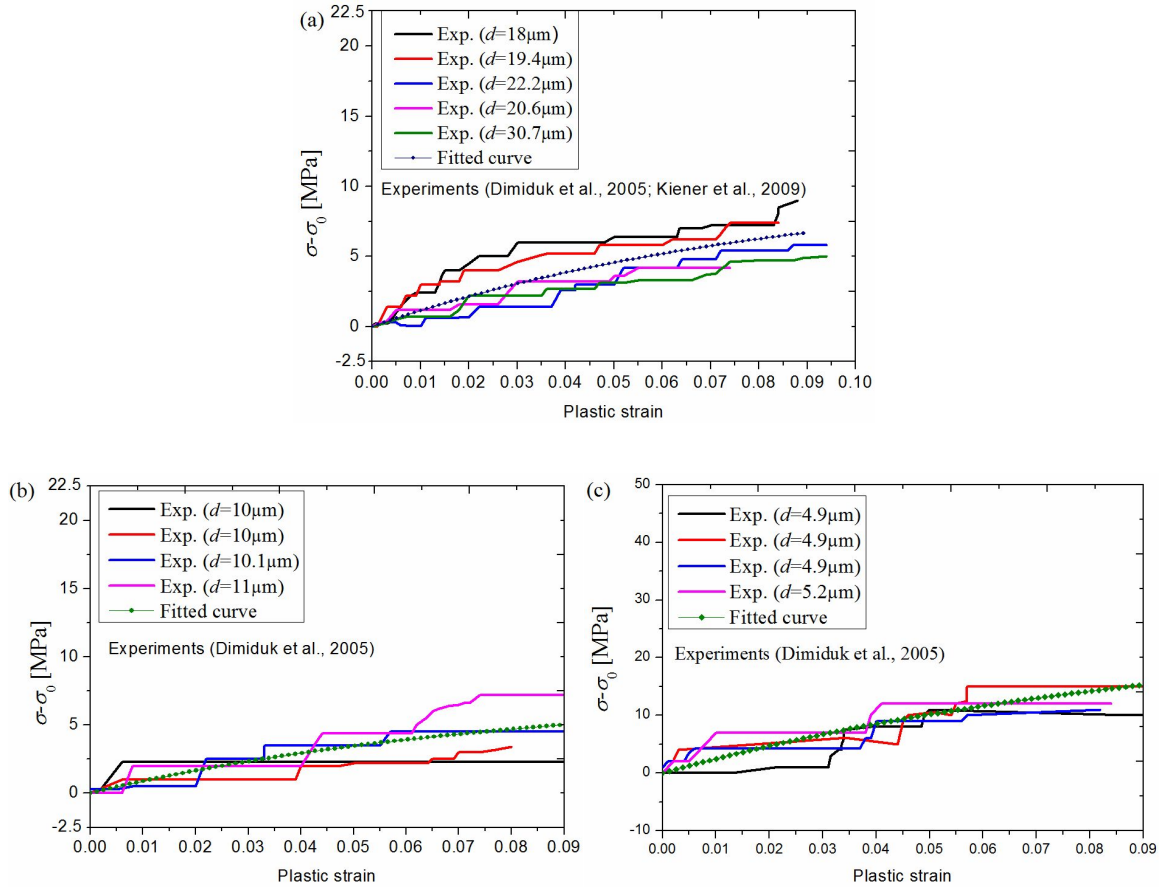


Fig. 1 Parameter determination of dislocation evolution from the experimental results of Ni with (a) diameter $d \sim 20 \mu\text{m}$, (b) $d \sim 10 \mu\text{m}$, and (c) $d \sim 5 \mu\text{m}$ (Dimiduk et al., 2005; Kiener et al., 2009).

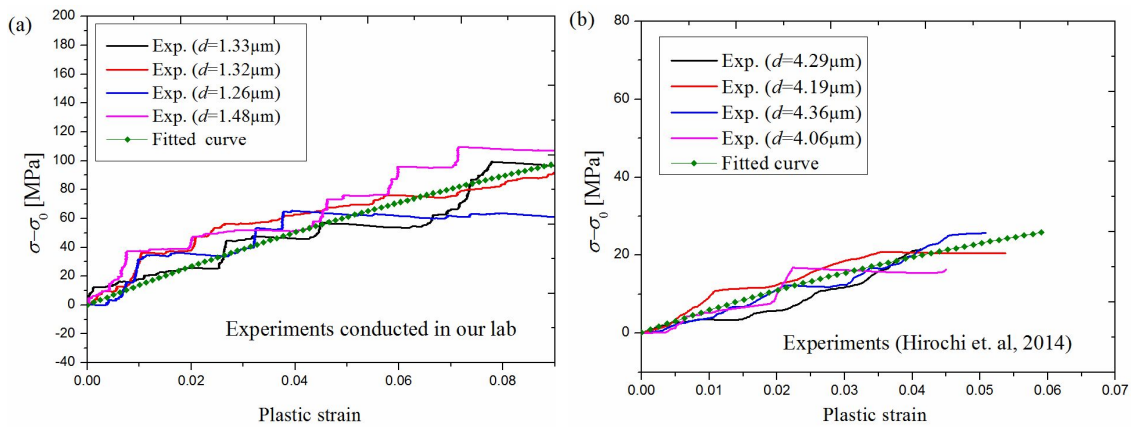


Fig. 2 Parameter determination of dislocation evolution from the experimental results of Cu with (a) diameter $d \sim 1 \mu\text{m}$ and (b) $d \sim 4 \mu\text{m}$ (Hirouchi and Shibutani, 2014).

Table 1 Dislocation evolution parameters fitted to experimental data.

	θ_y [MPa]	k^* [μm^{-1}]	Ω
Ni (5 μm)	276	56.2	20.3
Ni (10 μm)	85.7	45.6	25.6
Ni (20 μm)	129	47.1	23.3
Cu (1 μm)	1420	176	12.5
Cu (4 μm)	394	68.2	17.4

2.4 Hardening law accounting for the size effect in fcc pillars

For fcc metals, one commonly used phenomenological hardening law is the PAN model proposed by Peirce, Asaro, and Needleman (1982). According to the crystalline plasticity used in this study, the hardening modulus is given by

$$h_{\alpha\beta}(\gamma) = H_{\alpha\beta}(\gamma) + \frac{1}{2}(\beta^\beta : \mathbf{P}^\alpha - \beta^\alpha : \mathbf{P}^\beta), \quad (18)$$

where

$$\beta^\alpha = \mathbf{Q}^\alpha \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{Q}^\alpha, \quad (19)$$

and $\boldsymbol{\tau}$ is the Kirchhoff stress tensor. The symmetric tensor $\mathbf{P}^\alpha = \frac{1}{2}(\mathbf{s}_\alpha^* \otimes \mathbf{m}_\alpha^* + \mathbf{m}_\alpha^* \otimes \mathbf{s}_\alpha^*)$ and the skew-symmetric tensor $\mathbf{Q}^\alpha = \frac{1}{2}(\mathbf{s}_\alpha^* \otimes \mathbf{m}_\alpha^* - \mathbf{m}_\alpha^* \otimes \mathbf{s}_\alpha^*)$ are introduced here. $\mathbf{s}_\alpha$ and $\mathbf{m}_\alpha$ are the unity direction vector normal to slip plane and the unity sliding direction vector in the α sliding system. α, β is represented as the active slip system and $\mathbf{m}_\alpha^* = \mathbf{m}_\alpha \cdot \mathbf{F}_e^{-1}$, $\mathbf{s}_\alpha^* = \mathbf{F}_e \cdot \mathbf{s}_\alpha$, where $\mathbf{F}_e$ is the elastic deformation gradient tensor. In this model, the hardening matrix $H_{\alpha\beta}$ in Eq. (18) takes the form

$$H_{\alpha\beta}(\gamma) = H_{\beta\beta}(\gamma)[q + (1-q)\delta_{\alpha\beta}], \quad (20)$$

where

$$H_{\beta\beta}(\gamma) = H_0 \text{sech}^2\left(\frac{H_0\gamma}{\tau_s - \tau_0}\right) \text{ and } \gamma = \sum_{\alpha=1}^n |\gamma_p^{(\alpha)}|. \quad (21)$$

Here, q describes the latent hardening effect and is assumed to be 1.0 for coplanar and 1.4 for non-coplanar slip systems (Asaro and Lubarda, 2006). In this study, we chose $q = 1$ to describe the micropillars according to the recommendation of Zhang and Shang (2014). $H_{\alpha\beta}$ is a symmetric tensor, and in their model, H_0 is the initial hardening modulus, $n = 12$ for fcc materials, τ_0 is the initial value of the yield stress, and τ_s is the saturated shear stress at the stage of finite plastic deformation. A number of experimental compression tests on micropillars have found that their stress-strain curves appear to remain in the easy glide stage throughout the tests, and this is supported by the observation of postmortem transmission electron microscopy of nickel specimens (Norfleet et al., 2008). It thus seems to be appropriate to use the strain hardening model to characterize the experimental stress-strain curve. The PAN hardening laws for bulk materials have been widely discussed (Roters et al., 2010). However, there is no physical analysis of the hardening at the microscale.

In the PAN model, τ_0 and τ_s are provided by the experimental data without any physical parameters related to the size, and they cannot provide a physical understanding. The values of the current strength and the initial yield shear stress are provided in an appropriate way, such as based on experimental data or simulation definitions (Zhang and Shang, 2014; Gao et al., 2010). However, the hardening behavior in the micropillars is different from the bulk material, including multiplication of dislocations, boundary annihilation (Evers et al., 2004; Gurtin et al., 2000), and displacement burst (Zhang and Shang, 2014; Zhang et al., 2014). Here, we attempt to add the effect of dislocation evolution and size-dependent yield stress into the hardening model.

In the PAN hardening model, τ_s is the saturated shear stress at the stage of finite plastic deformation. If we replace τ_0 and τ_s by τ_{SAS}^0 and τ_{SAS}^f , τ_{SAS}^f should be the saturated shear stress of the micropillars, and then $\varepsilon_p = \varepsilon_s$, where ε_s is the strain corresponding to τ_s . The revised form of the PAN hardening model can be written as

$$H_{\beta\beta}(\gamma) = H_0 \text{sech}^2\left(\frac{H_0\gamma}{\tau_{\text{SAS}}^f - \tau_{\text{SAS}}^0}\right). \quad (22)$$

where

$$\tau_{\text{SAS}}^f - \tau_{\text{SAS}}^0 = 0.5\mu b \left[\left(\varepsilon_p / bn \right)^2 + \frac{1}{\Omega^2} \left\{ k^* - \frac{k^* - \Omega\sqrt{\rho_0}}{\exp(\Omega\varepsilon_p / 2)} \right\}^2 \right]^{0.5} - 0.5\mu b\sqrt{\rho_0}. \quad (23)$$

In Eq. (23), the hardening model includes the dislocation evolution parameters (those are k^* and Ω). The initial yield stress is replaced by τ_{SAS}^0 , which can express the size-dependent properties.

The difference between τ_{SAS}^0 and τ_{SAS}^f in Eq. (23) is shown in Fig. 3. When $R > 10 \mu\text{m}$, the difference between τ_{SAS}^0 and τ_{SAS}^f is nearly constant. Relating this to Eq. (23), it can be determined that the hardening modulus is size independent when the diameter is sufficiently large. In this range, the original PAN hardening model without considering the size effect is reasonable. However, if $R < 10 \mu\text{m}$, the size-dependent difference of τ_{SAS}^0 and τ_{SAS}^f makes the hardening modulus size-dependent.

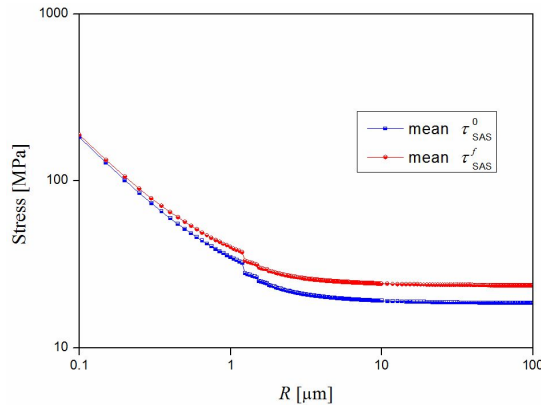


Fig. 3 Comparison of τ_{SAS}^0 and τ_{SAS}^f for different R values.

From Eqs. (22) and (23), the hardening modulus is related to the dislocation evolution parameters. The parameters are selected from the articles of Beyerlein and Tomé (2008), Pan et al. (2015), and Parthasarathy et al., (2007), and they are given in Table 2. Figure 4 shows that the hardening modulus of Cu is affected by the characteristics of dislocation evolution by k^* and Ω . The parameters of the original PAN model are $H_0 = 56.8 \text{ MPa}$, $\tau_0 = 41.1 \text{ MPa}$, and $\tau_s = 1.53\tau_0$ (Zhang et. al., 2014). In Fig. 4(a), the original PAN hardening model is compared with the revised PAN hardening model with different k^* and $\Omega = 17.4$. Figure 4(b) shows the hardening modulus of Cu with different Ω values and $k^* = 68.2 \mu\text{m}^{-1}$. The dislocation evolution parameters result in different hardening modulus, as shown in Fig. 4. As shown in Table 1, k^* and Ω are size dependent. That is, the hardening modulus should be different to account for the different size by using different values of k^* and Ω .

Table 2 Parameters used in the extended SAS model and CPFE model.

Parameters	Values	Parameters	Values
$\rho_0 [\text{m}^{-2}]$	2×10^{12}	$b [\text{nm}]$	0.255
τ_0 in Eq. (10) [MPa]	12	$k^* [\mu\text{m}^{-1}]$	176 ($d = 1 \mu\text{m}$) 68.2 ($d = 4 \mu\text{m}$)
$\mu [\text{GPa}]$	48	Ω	12.5 ($d = 1 \mu\text{m}$) 17.4 ($d = 4 \mu\text{m}$)
ν	0.3		

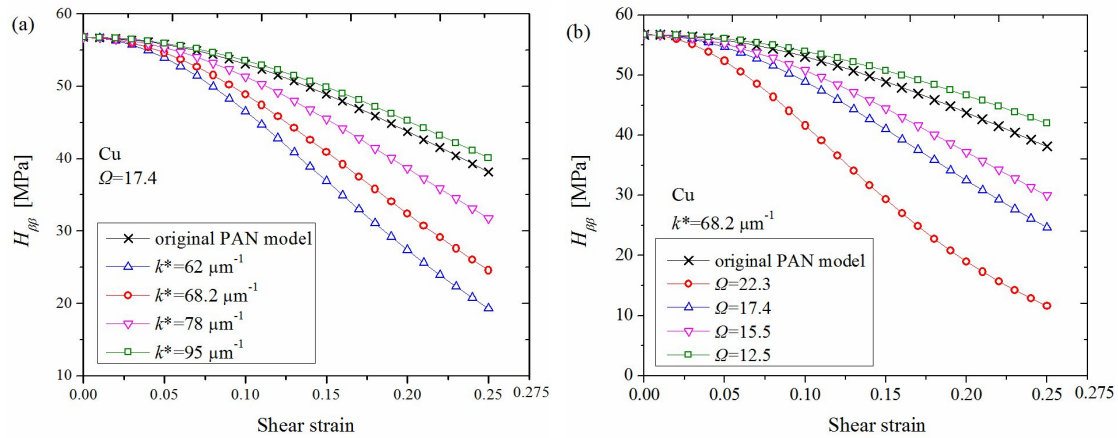


Fig. 4 Effect of dislocation evolution on the hardening modulus for (a) different k^* and (b) different Q .

3. Finite element model of Cu micropillar compression test

We performed finite element (FE) analyses using a user material subroutine (UMAT) in the commercial code ABAQUS/Standard (2012). In UMAT, initial yield stresses and subsequent yield stresses, which are introduced in Section 2.2, and the present redefined hardening model, which is introduced in Section 2.4, are implemented in the CPFE framework. The normal micropillar axes are set to the $[6\ 11\ 5]$ and $[6\ 1\ 5]$ surface orientations, which are the same as those used by Hirouchi and Shibutani (2014). In the calculations, we performed the compression tests with a flat punch, which is treated as the rigid body, as shown in Fig. 5. In addition, isothermal conditions were assumed and the specimens were kept at room temperature. Pillars with diameters of 1 and 4 μm were simulated, and the height-to-diameter aspect ratio was fixed at 2.5 in all of the simulations. For simplicity, the FE model consisted of a single 8-node brick-type element (C3D8). The displacements were applied along the y direction associated with a constant strain rate of $1.0 \times 10^{-4} \text{ s}^{-1}$. A base material at the bottom of the pillar was included to simulate to the real boundary condition of the samples.

The material parameters used in the simulations are given in Table 2. The elastic moduli (Freund and Suresh, 2003) and the related parameters of the FEM simulations are given in Table 3. The CRSS was chosen as τ_{SAS}^0 in Eq. (9), which is dependent on the scale. The initial hardening moduli H_0 was determined using a similar approach to a previously published method (Zhang and Shang, 2014; Zhang et al., 2014).

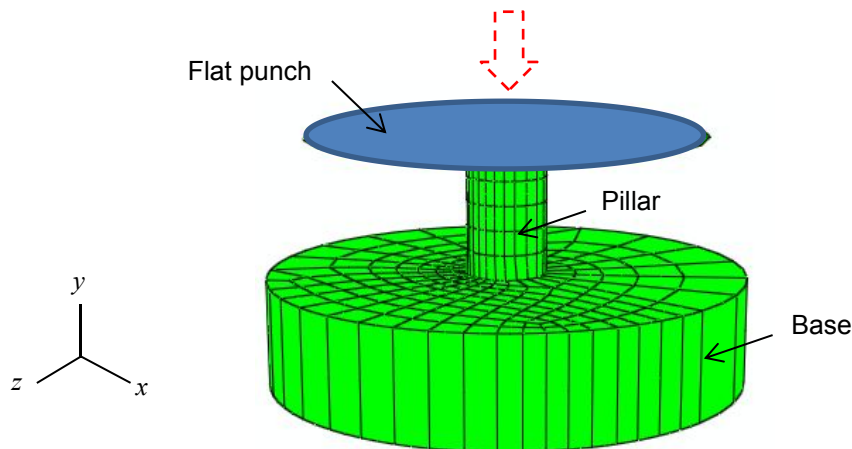


Fig. 5. Finite element model of micropillar and the boundary conditions.

Table 3 CPFE parameters.

Parameters	Values
c_{11} [GPa]	168.4
c_{12} [GPa]	121.4
c_{22} [GPa]	75.4
ε_s	0.3
H_0 [MPa]	283.8 ($d = 1 \mu\text{m}$), 78.5 ($d = 4 \mu\text{m}$)

4. Results and discussion

4.1 Stress–strain responses

Figure 6 shows the relationship between compressive stress and plastic strain obtained from the FEM simulations using the original PAN hardening model and the revised PAN hardening model. Because the size-dependent yield stress is based on the initial distribution of dislocations, the initial yield stress might not agree well with the experimental results. Therefore, we compare the net stress $\sigma - \sigma_{\text{SAS}}^0$. Compression of Cu pillars was performed for the samples with diameters of $d \sim 4 \mu\text{m}$ for the $[6\ 1\ 5]$ surface axis and $d \sim 1 \mu\text{m}$ for the $[6\ 1\ 5]$ surface axis using the dislocation evolution parameters $k^* = 68.2 \mu\text{m}^{-1}$ and $\Omega = 17.4$, and $k^* = 176 \mu\text{m}^{-1}$ and $\Omega = 12.5$, respectively. The original PAN hardening model chooses $\tau_s = 1.53\tau_0$ (Zhang et al., 2014). In Fig. 6, the flow stress of the original PAN hardening model is almost the same as that of the revised PAN hardening model when the strain is small. However, the flow stress of the original PAN hardening model is larger than that of the revised PAN hardening model when the strain is large. The reason is that the original PAN hardening modulus is much larger than the revised PAN modulus when the strain is large, as shown in Fig. 4. Compared with the curves of revised PAN model in Figs. 6(a) and (b), the flow stresses are quite different because of the different sets of k^* and Ω , as shown in Fig. 4.

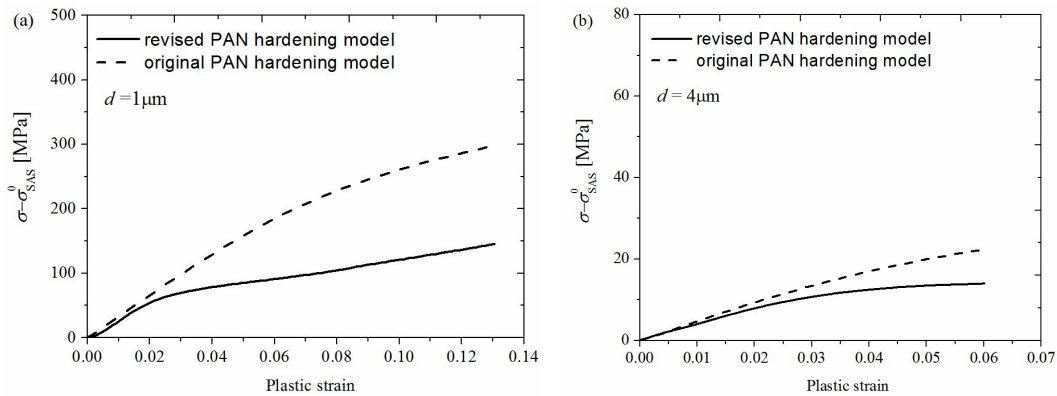


Fig. 6 Comparisons of the hardening flows between the revised PAN and the original PAN models for the compression tests of $[6\ 1\ 5]$ and $[6\ 1\ 5]$ copper pillars with diameters of (a) $1 \mu\text{m}$ and (b) $4 \mu\text{m}$, respectively.

In the CPFE model, size-dependent hardening is dominated by the dislocation-based hardening model (Eq. (22)). In Fig. 2, the hardening flows of the experiments show several bursts, which have been studied by the FEM analyses (Zhang and Shang, 2014). However, it is very hard to determine the time when a displacement burst will occur and the magnitude of the displacement burst. How to provide the exact response considering such a displacement is still an open issue, which needs more investigation. In this study, the average value of the plastic response is used for discussion.

Figure 7(a) shows the stress–strain responses with different k^* values and $\Omega = 17.4$. The stress with a high k^* value is larger than that with a small k^* value. Compared with Fig. 4(a), a higher hardening modulus results in a larger stress–strain response. Similar results were obtained with different Ω values and $k^* = 68.2 \mu\text{m}^{-1}$ because the larger stress–strain response is dominated by the hardening modulus (see Fig. 7(b)).

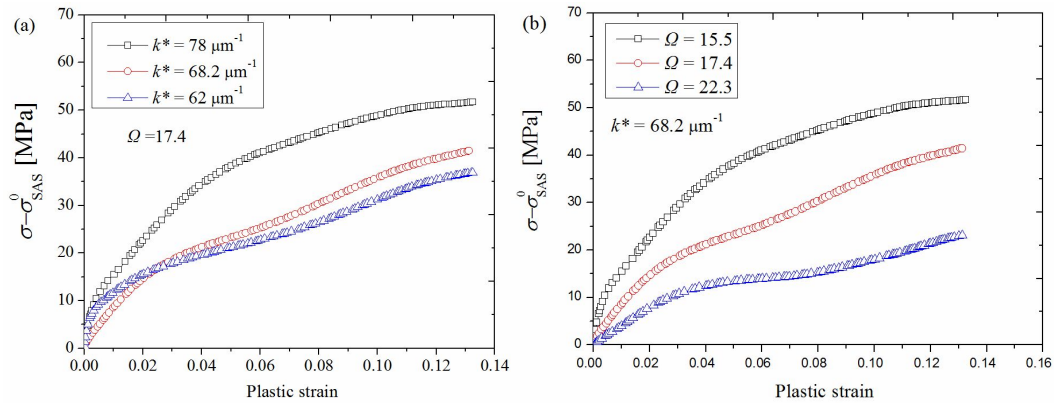


Fig. 7 Dislocation evolution effect on hardening for (a) different k^* and (b) different Ω .

4.2 Shear deformations inside the pillar

Figure 8 shows a comparison of the scanning electron microscopy (SEM) image of the compressed pillar with the crystalline orientation $[6\ 11\ 5]$ and the FEM deformed mesh image. In the FEM deformed image, the color represents the scaled magnitude of displacement in the micropillars for displaying. The slip band in the SEM image has an angle of around 50° with respect to the normal axis and occurs along the $(1\ 1\ \bar{1})\ [0\ 1\ 1]$ slip plane, which is the crystalline system with the maximum Schmid factor (Hirouchi and Shibutani, 2014). The deformation band is similar to the experimental results of Hirouchi and Shibutani (2014).

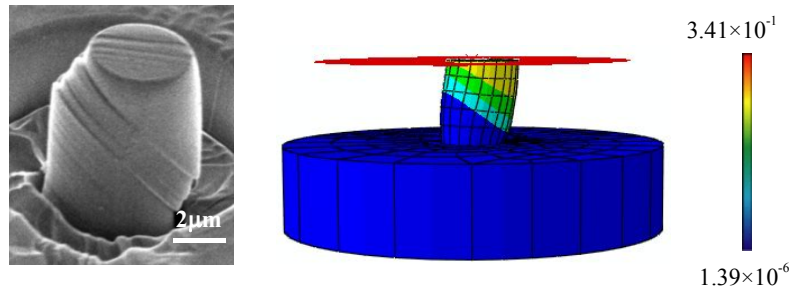


Fig. 8 Comparison of the SEM image and the FEM deformed mesh image (displacement image) at normal compressive strain of $\varepsilon = 0.134$. The color of the FEM image indicates the scaled magnitude of displacement in the micropillar.

Figures 9 and 10 show the shear strains $\gamma_p^{(\alpha)}$ in Eq. (21) on 12 slip planes with crystalline orientations of $[6\ 11\ 5]$ and $[6\ 1\ 5]$, respectively. In Fig. 9, the $(1\ 1\ \bar{1})\ [0\ 1\ 1]$ slip plane has the maximum Schmid factor (0.431) and the maximum shear strain. The shear band is clear and the same as the experimental SEM image in Fig. 8. In Fig. 9, there is a shear strain on the $(1\ 1\ 1)\ [0\ \bar{1}\ 1]$ slip plane with the Schmid factor 0.296. Compared with shear strain on the $(1\ 1\ \bar{1})\ [0\ 1\ 1]$ slip plane, its shear strain is smaller than that of the system. In other words, the shear deformation is uniformly distributed on the slip plane with the maximum Schmid factor. A similar phenomenon is seen in Fig. 10. In Fig. 10, the $(1\ \bar{1}\ 1)\ [1\ 1\ 0]$ slip plane has the maximum Schmid factor (0.461) and the maximum shear strain. Strain localization can also be found on the slip plane with the second largest Schmid factor (0.395), but the value is much smaller than that on the $(1\ \bar{1}\ 1)\ [1\ 1\ 0]$ slip plane. In summary, the shear band in the micropillar is mainly on the slip plane with the largest Schmid factor. The shear strains on the other slip planes can also be found because the crystal orientation would change during deformation, but they are still small.

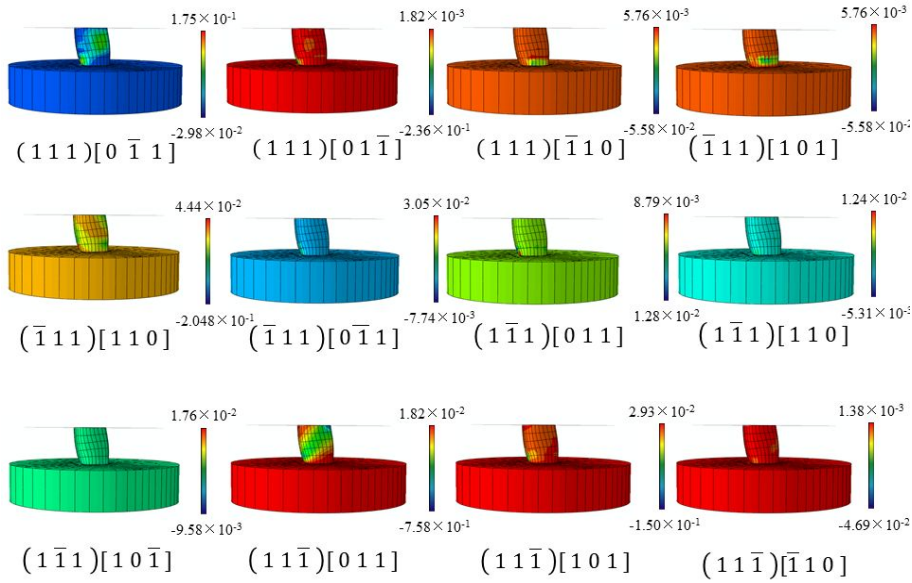


Fig. 9 Shear strains $\gamma_p^{(\alpha)}$ in Eq. (21) on different slip planes with orientation of $[6\ 11\ 5]$ at normal compressive strain of $\varepsilon = 0.134$.

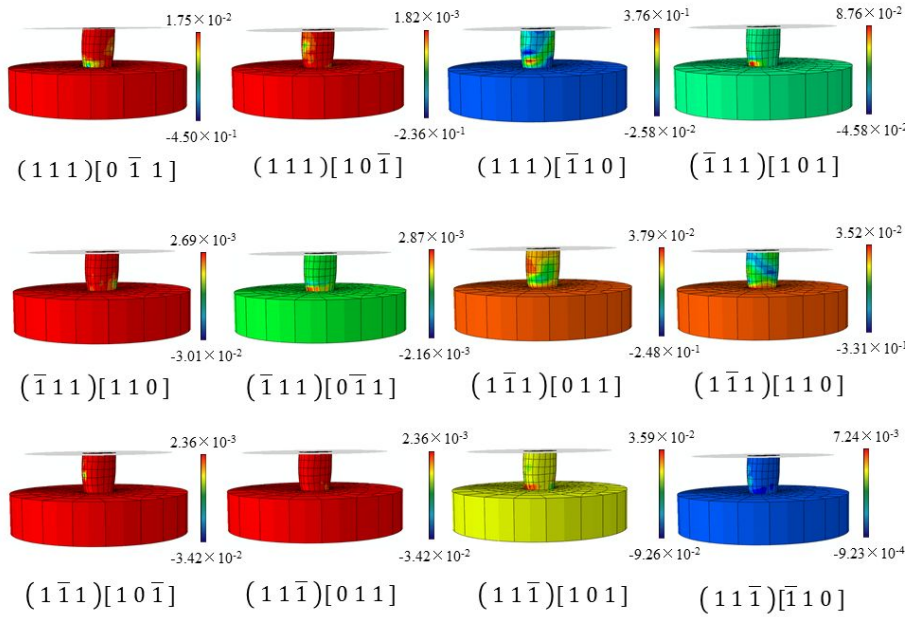


Fig. 10 Shear strains $\gamma_p^{(\alpha)}$ in Eq. (21) on different slip planes with orientation of $[6\ 1\ 5]$ at normal compressive strain of $\varepsilon = 0.134$.

4.3 Friction effect on shear band and hardening

Most of the previous simulations of micropillars (Gerken and Dawson, 2008; Zhang and Shang, 2014; Zhang et al., 2014) did not include the friction between the flat punch and the top surface of the pillar. Shear deformation inside the pillar with the non-friction condition was discussed in Section 4.2. As mentioned before, the shear band in the micropillar was mainly on the slip system with the maximum Schmid factor. If the friction effect is considered in the model, the deformed image of the pillar with $[6\ 11\ 5]$ surface orientation in Fig. 11 also shows the shear band, which is slightly different from that in Fig. 8. Figure 12 shows the distribution of the nonzero shear strains in the slip planes with the largest three Schmid factors, and the information about the slip systems is given in Table 4. Except for the slip planes shown in Fig. 12, the shear strains on the other slip planes are almost zero. In Fig. 12, the local slip deformations

in green or light blue on the #5, #10, and #11 slip planes are activated by external compression. In Fig. 9, the shear strain is only on the slip plane with the maximum Schmid factor. However, the shear band shown in Fig. 11 is due to multiple slip planes.

The friction between the flat punch and the top surface of the pillar makes the local deformation near the punch different from that in the middle of the pillars (Dimiduk et al., 2005; Uchic et al., 2004). Accompanied by global plastic strain, dislocations near the punch would pile up and climb from the maximum Schmid factor slip plane to the other slip planes (Gerken and Dawson, 2008; Pan et al., 2015), which are the green parts near the punch on the #5 and #11 slip planes shown in Fig. 12. The constrained deformation resulting from the local dislocation pile-up and climb makes the external compression activate the other slip planes. Because the dislocations on the slip plane with maximum Schmid factor might move to the surface and form the single slip bands shown in Fig. 8, the non-friction case in this study is reasonable.

Table 4 Slip system in FEM Simulation

#	slip plane	slip direction	SF with friction	SF without friction
1	(1 1 1)	[0 $\bar{1}$ 1]	-0.296	-0.296
2	(1 1 1)	[1 0 $\bar{1}$]	0.049	0.049
3	(1 1 1)	[1 1 0]	0.247	0.247
4	(1 1 1)	[1 0 1]	0.222	0.222
5	($\bar{1}$ 1 1)	[1 1 0]	0.343	0.343
6	($\bar{1}$ 1 1)	[0 $\bar{1}$ 1]	-0.121	-0.121
7	(1 $\bar{1}$ 1)	[0 1 1]	0	0
8	(1 $\bar{1}$ 1)	[1 1 0]	0	0
9	(1 $\bar{1}$ 1)	[1 0 1]	0	0
10	(1 1 $\bar{1}$)	[0 1 1]	0.431	0.431
11	(1 1 $\bar{1}$)	[1 0 1]	0.296	0.296
12	(1 1 $\bar{1}$)	[$\bar{1}$ 1 0]	0.134	0.134

Red words represent the active slip systems

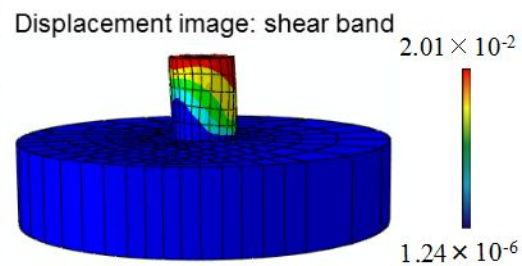


Fig. 11 Slip system and displacement deformed shear band image at normal compressive strain of $\varepsilon = 0.134$.

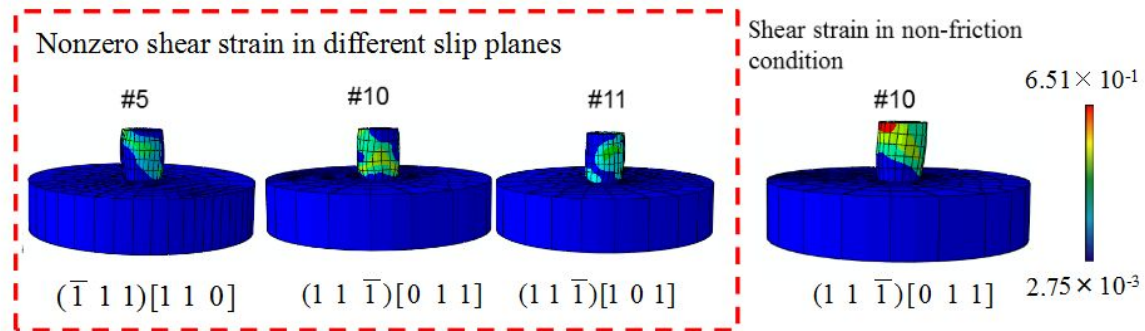


Fig. 12 Friction effect on shear deformation on the slip plane at normal compressive strain of $\varepsilon = 0.134$.

Figure 13 shows the results of the stress-strain responses of the pillars with Coulomb's friction model. The friction coefficient f was set to 0, 0.3, or 0.5. The results show that the hardening stress versus plastic strain curve is steeper for the largest friction coefficient ($f = 0.5$) than without friction ($f = 0$). In the friction case, constrained deformation resulting from local dislocation pile-up and climb makes the external compression activate the other slip planes. According to the Schmid law of $\tau^\alpha = P^\alpha : \sigma$, the shear stress τ^α on a slip plane with small a Schmid factor needs a larger external stress than that with the maximum Schmid factor. Moreover, dislocation pile-up and climb alter the crystalline structure and even distort the crystal lattice, and this increases the $h_{\alpha\beta}$ term in Eq. (18). The distorted crystal lattice results in the multiple slip planes being activated when the plastic strain is generated. However, activating and generating multiple slip planes requires more stress, which represents more obvious hardening (Asaro and Lubarda, 2006; Gao et al., 2010). The experiments also show that multiple slips are more difficult than a single slip (Hirouchi and Shibutani, 2014). To understand this phenomenon, the effect of friction on the hardening modulus $h_{\alpha\beta}$ is shown in Fig. 14. The results show that the $h_{\alpha\beta}$ value in the simulation considering friction is larger than the value without friction,

and $h_{\alpha\beta}$ for the large friction coefficient ($f = 0.5$) is larger than that for the small friction coefficient ($f = 0.3$). This means that the hardening stress with a large friction coefficient would be large, which agrees with the results shown in Fig. 13.

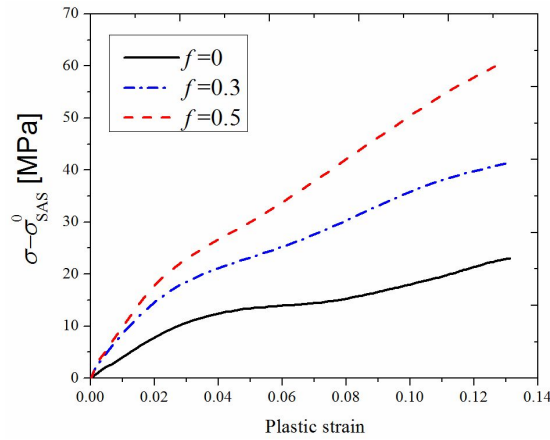


Fig. 13 Effect of friction on the hardening stress of micropillars with the crystalline orientation [6 11 5].

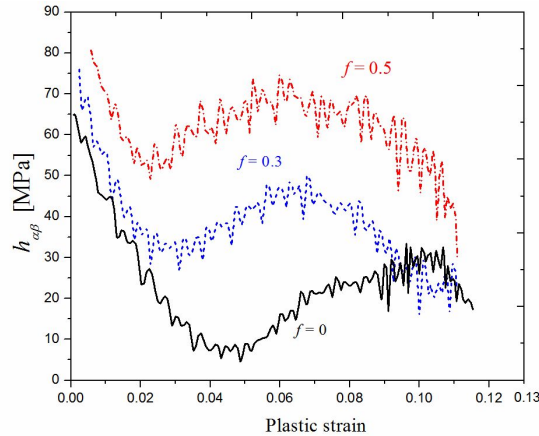


Fig. 14 Friction effect on the hardening modulus. The friction between the punch and the pillar constrains rotation of the pillar, which affects the hardening flow increments during the simulation.

5. Conclusions

In this study, we propose a physical constitutive model with the framework of the CPFE method that accounts for the dislocation physics to describe the size-dependent plastic deformation of micropillars. To predict the variation of the plastic state owing to size-dependent internal microstructures, such as dislocation sources, dislocation source length, mobile dislocations, and trapped dislocations, information about these defects is introduced by providing dislocation evolution based on the Orowan equation and the principle of Bergstrom dislocation evolution, and the extended SAS model. Our conclusions are as follows:

- (1) The present formulation suggests that the dislocation evolution equation includes both mobile dislocations and trapped dislocations, and the total dislocation density is a function of the plastic strain, the number of dislocation sources, and the dislocation evolution parameters.
- (2) Based on the SAS model, a revised PAN hardening model is proposed that can describe size-dependent hardening flow.
- (3) The physical constitutive equations combined with the SAS model, the revised PAN hardening model, and CPFE framework can describe the size-dependent plastic flow of micropillars.

(4) Size-dependent dislocation evolution is related to the hardening modulus of the micropillars, and this makes the stress–strain response vary with the micropillar size.

(5) The friction between the flat punch and the top surface of the pillar affects the stress–strain response of the plastic flow and the shear band deformation of the micropillars. Hardening with friction is greater than that under the non-friction condition. Friction makes the shear strain on the slip plane much more complicated.

Acknowledgements

The ABAQUS subroutine UMAT used here is a modified version written by Prof. Yonggang Huang and Prof. Jeffrey W. Kysar. Y. Shibutani gratefully acknowledges financial support from Grants-in-Aid for Scientific Research (A) (26249002) and H. Tanaka thanks Young Scientists (A) (25709001) for financial support.

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