Arch. Mech., 52, 1, pp. 103–125, Warszawa 2000

A new approach to the analysis of polycrystal plasticity

X. PENG and J. FAN

Department of Engineering Mechanics, Chongqing University, Chongqing, 400044, P. R. China

WHEN A POLYCRYSTAL IS SUBJECTED TO INELASTIC deformation, there inevitably exist residual microstress fields in a *polycrystalline material* due to its nonhomogeneous morphology. The energy stored in these microstress fields may partly be released and influence the material behavior during subsequent inelastic deformation. Correspondingly, a simple mechanical model is introduced to formulate the constitutive equation for a slip system and the hardening law for single crystal. The corresponding approach for the analysis of polycrystalline materials is obtained based on KBW's self-consistent theory. The proposed approach employs no yield criterion and the corresponding numerical analysis is greatly simplified because it involves no additional process for determination of the activation of slip systems and slip direction. A mixed averaging approach is used in polycrystalline plasticity analysis. The response of 316 stainless steel subjected to typical biaxial nonproportional plastic strain cycling is described and the validity of the proposed approach is demonstrated by the satisfactory agreement between the calculated result and experimental observation.

Key words: Crystal plasticity, Hardening law, Nonproportional cyclic plasticity of Polycrystal

1. Introduction

THE RESEARCH ON CRYSTAL plasticity can be dated back to 1930's [1]. Since HILL [2], HILL and RICE [3] built up a complete system of the geometry and kinetics of crystal plasticity, it becomes more and more attractive.

The conventional constitutive relation of a slip system was derived within the framework of the conventional theory of plasticity, i.e., taking the existence of a yield shear stress as its basic premise. Suppose a single crystal is subjected to the stress σ_c, the activation of its ith slip system is determined by [4]

$$\gamma^{(1)} \begin{cases} \geq & \text{if} \quad \sigma_c : \mathbf{a}^{(1)} = \tau^{(1)} \quad \text{and} \quad \sigma_c : \alpha^{(1)} = \dot{\tau}^{(1)}, \\ = 0 & \text{if} \quad \sigma_c : \alpha^{(1)} < \tau^{(1)} \text{ or } \sigma_c : \alpha^{(1)} = \tau^{(1)} \\ & \qquad\qquad\qquad\qquad \text{while } \sigma_c : \alpha^{(1)} < \dot{\tau}^{(1)}, \end{cases} \tag{1.1}$$

where

$$\alpha^{(1)} = \frac{1}{2}\left(\mathbf{n}^{(1)} \otimes \mathbf{s}^{(1)} + \mathbf{s}^{(1)} \otimes \mathbf{n}^{(1)}\right) \tag{1.2}$$

denotes the orientation tensor of the slip system, $\mathbf{n}^{(i)}$ and $\mathbf{s}^{(i)}$ are the unit vectors directed along respectively along the outer normal of the slip plane and in the slip direction. In general, the hardening law of a single crystal can be expressed as

$$\dot{\tau}^{(1)} = \sum_{j=1}^{N} h_{ij}\dot{\gamma}^{(1)} \tag{1.3}$$

where h_{ij} denotes the hardening coefficient. Some kinds of h_{ij} have been proposed on the basis of different kinds of hardening mechanisms [5 – 10].

In the existing literature analyzing polycrystalline response, additional iterations were usually introduced to determine the activation of slip systems and slip direction because of the existence of a critical shear stress and the corresponding slip criterion (see Eq. (1.1)). This not only increases the complexity, but also affects the efficiency and accuracy in the corresponding computational process. In the analysis under a plastic strain controlled process, the computation becomes more complicated.

A constitutive equation for a slip system is derived on the basis of on a simple mechanical model, which enables to obtain the hardening law for a single crystal and the corresponding analysis for polycrystalline response based on KBW's self-consistent theory. Since the proposed model employs no yield criterion so that no additional iteration is used for the determination of the activation of slip systems and the direction of slip, great convenience is experienced in the analysis of polycrystalline plasticity. The response of 316 stainless steel subjected to plastic strain cycling along typical paths in biaxial plastic strain plane is analyzed and the validity of the proposed approach is demonstrated by the satisfactory agreement between the theoretical and the experimental results [11].

2. Constitutive equation for single crystal

In polycrystalline materials, the deformation of any single crystal is inevitably constrained by the neighboring crystals due to the nonhomogeneous morphology of the materials, which may lead to residual microstress fields when plastic deformation occurs. On the other hand, when plastic deformation occurs in a single crystal, there also exist residual microstress fields in the stochastic microstructures due to the nonhomogeneous nature and the respective pattern of lattice defects, for instance, residual distortion, dislocation and its substructures, etc.

[12]. The energy stored in these microstress fields may partly be released under certain condition, which reduces the external energy needed for further plastic deformation of the crystals. Correspondingly, a simple mechanical model (see Fig. 1) is introduced to describe the constitutive behavior of a slip system, the similar concept of which was also used in other papers [13 – 15].

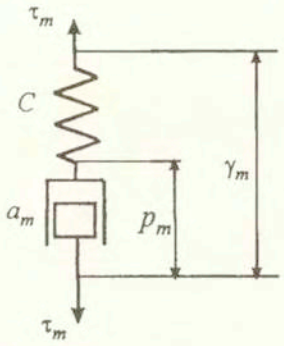

FIG. 1. A simple mechanical model for the constitutive relation of a slip system.

It is seen in Fig. 1 that the dissipated mechanism of the mth slip system is described by a dashpot-like block a_m (with plastic damping coefficient a_m) and a spring C (with stiffness C). The latter is related to the stochastic internal structure, and the energy stored in the spring C represents the energy stored in various kinds of the residual microstress fields. The deformation of the spring C represents the part of plastic deformation (slip) that may recover under some condition and does not make any contribution to the macroscopic elastic property. $p^{(m)}$, the deformation of a_m, is an internal variable that represents the irreversible part of the deformation on the mth slip system. The behavior of the spring is described by

$$\tau^{(m)} = C\left(\gamma^{(m)} - p^{(m)}\right) \qquad m = 1, 2, ..., N, \tag{2.1}$$

where $\gamma^{(m)}$ and $\tau^{(m)}$ denote the strain and the shear stress on the mth slip system, N is the number of the independent ones. The change of $p^{(m)}$ and the corresponding $\tau^{(m)}$ should satisfy the dissipation inequality $\tau^{(m)} dp^{(m)} \geq 0$ (m not summed). By introducing a generalized time $\zeta^{(m)}$ defined by

$$d\zeta^{(m)} = \left| d\gamma^{(m)} \right|. \tag{2.2}$$

$\tau^{(m)}$ can be assumed to satisfy the following phenomenological relation:

$$\tau^{(m)} = a_m \frac{dp^{(m)}}{d\zeta^{(m)}}, \quad (m \text{ not summed}), \tag{2.3}$$

where $a_m > 0$ so that the dissipation inequality can be satisfied in any case. During irreversible deformation, obstacles formed by the pile-ups and tangles of dislocations increase the resistance to active dislocations and result in macroscopic hardening. The hardening of the mth slip system can phenomenologically be described by the change of a_m. Suppose the hardening can be separated into instantaneous hardening and cross-hardening related respectively to the slip on a single slip system and the interaction between the slips on different slip systems [10], which are represented respectively by f_m and H_m, and assuming

$$a_m = a_0 f_m H_m \qquad dz^{(m)} = \frac{d\zeta^{(m)}}{f_m H_m} \quad (m \text{ not summed}), \tag{2.4}$$

Eq. (2.3) can be rewritten as

$$\tau^{(m)} = a_0 \frac{dp^{(m)}}{dz^{(m)}} \quad (m \text{ not summed}), \tag{2.5}$$

in which a_0 is the initial plastic damping coefficient and $z^{(m)}$ is the generalized time scale of the mth slip system. By combining Eqs. (2.1), (2.3) and (2.4), one obtains

$$d\tau^{(m)} = C d\gamma^{(m)} - \alpha \tau^{(m)} dz^{(m)} \quad (m \text{ not summed}) \tag{2.6}$$

in which $\alpha = \dfrac{C}{a_0}$. If $C \to \infty$, then $p^{(m)} = \gamma^{(m)}$ (see Fig. 1), and one obtains immediately the following result from Eqs. (2.5) and (2.6)

$$\tau^{(m)} = \pm a_0 f_m H_m \quad (m \text{ not summed}). \tag{2.7}$$

It is just the critical condition in the constitutive relation of the conventional crystal plasticity, in which a_0 is the initial critical shear stress. It should be stressed that the component C (see Fig. 1) is related to stochastic internal microstructure and makes no contribution to the macroscopic elastic shear modulus G (see Sec. 4). Eq. (2.6) is, therefore, a relation to describe the slip (instead of overall elastoplastic deformation) on the mth slip system. The form of Eq. (2.6) is similar to a single term in the endochronic model [16], the back stress proposed by CHABOCHE [17] and some other constitutive equations. The proposed model does not use a yield criterion, but it can include the conventional relation with a yield criterion as its special case (see Eq. (2.7)). It can also be proved that there exists a limit in stress when slip fully develops [18]. The introduction of the stored energy may, on the one hand, make the slip model more realistic, and on the other hand, make the analysis for polycrystalline response much more convenient.

For easier application to crystal plasticity, Eq. (2.6) can further be expressed as

$$\dot{\tau}^{(m)} = T_m \dot{\gamma}^{(m)} \quad (m \text{ not summed}), \tag{2.8}$$

where

$$T_m = C - \frac{\alpha \Gamma_m}{f_m H_m}, \qquad \Gamma_m = \frac{d\gamma^{(m)}}{d\zeta^{(m)}} \quad (m \text{ not summed}), \tag{2.9}$$

By defining the following hardening coefficient

$$h_{mn} = T_m \delta_{mn} \quad (m \text{ not summed}), \tag{2.10}$$

one obtains the hardening law for a single crystal

$$\dot{\tau}^{(m)} = \sum_{n=1}^{N} h_{mn} \dot{\gamma}^{(n)} \quad (m = 1, 2, ..., N). \tag{2.11}$$

It is easily found that for non-softening materials, h_{mn} is positive definite, which guarantees the existence and uniqueness of the solution. The above relations will be used in the following analysis for the nonproportional cyclic plasticity of 316 stainless steel.

It should be mentioned that although the form of the definition of h_{mn} in Eq. (2.10) is similar to Koiter's postulate of independent hardening [19], the interactive hardening can be considered through H_m. Bassani once mentioned that the least well-characterized aspect of the constitutive framework for either time-dependent or independent behavior is the set of instantaneous hardening moduli h_{mn} that relate the rate of hardening on each slip system to the plastic slip-rate on all systems [10]. If H_m is assumed in the following form

$$H_m^{-1} = \sum_{n=1}^{N} g_{mn} \frac{\dot{\zeta}^{(n)}}{\dot{\zeta}^{(m)}}, \tag{2.12}$$

one obtains the hardening coefficients (see Eq. (2.11)) as follows:

$$h_{mn} = C\delta_{mn} - \frac{\alpha \tau^{(m)}}{f_m} g_{mn} \Gamma, \quad (m, n \text{ not summed}), \tag{2.13}$$

where δ_{mn} denotes the Kronecker symbol and g_{mn} is a set of material-, geometry-, temperature- and plastic deformation history-dependent parameters. The form of the obtained relation is similar to that taking into account the latent hardening. It is easily found that for non-softening materials, a conservative result is that if g_{mn} is selected so that $f_m H_m$ is non-decreasing during any plastic deformation process, h_{mn} will be positive definite, which guarantees the existence and uniqueness of the solution. If $g_{mn} = 0$ for $m \neq n$ then the h_{mn} in Eq. (2.13) reduces to that in Eq. (2.10).

3. Physically based hardening functions

In Eq. (2.4) the hardening functions f_m and H_m are introduced to describe respectively the hardening related to single slip and cross-hardening related to the interaction between the slips on different slip systems.

Although the hardening mechanisms may be complicated during the plastic deformation process, dislocation pile-ups and tangles are considered to be the two dominant ones.

Dislocation pile-ups form obstacles against active dislocations. The associated long-range microstress fields are directional and thus kinematic, which can account to some extent for the Bauschinger effect. The hardening of a slip system induced by dislocation pile-ups should be determined by the superimposition of the effects of the corresponding residual microstress fields caused by the dislocations pile-ups in all slip systems.

The hardening induced by dislocation tangles is attributed to the interaction between the active dislocations and dislocation forests. The associated residual microstress field is short-ranged and less directional. This type of hardening strongly depends on the slip histories and the current states of dislocations at all slip systems. The interaction between dislocations on different slip systems may result in different hardening effects. The corresponding description should, therefore, be able to express its history-dependence and the different effect caused by the interaction between different slip systems.

The hardening behavior of materials strongly depends on the current microstructure of the materials, but macroscopically described by the hardening functions. Suppose f_m possesses a saturated value corresponding to the saturated state of dislocation when plastic deformation fully develops, the evolution of f_m can be determined by

$$\frac{df_m}{dz^{(m)}} = \beta_1(d_1 - f_m), \tag{3.1}$$

where d_1 and β_1 are two material-dependent parameters representing respectively the saturation value of f_m and the rate for f_m to approach d_1.

BASSANI [10] proposed a hardening law that can well describe cross-hardening based on a detailed analysis. This law is directly adopted to be the cross-hardening function H_m as follows

$$H_m = 1 + \sum_{k \neq m} f_{mk} \mathrm{th}(2\beta_s \zeta^{(k)}) \quad (m = 1, 2, ..., N), \tag{3.2}$$

in which $\zeta^{(k)}$ denotes the accumulated slip at the kth slip system, β_s is a material parameter representing the rate for H_m to approach to its saturation value, and f_{mk} denote coupled hardening coefficients connecting the relative orientation of

the considered two slip systems m and k, which can take into account the contribution of the accumulated slip of the kth slip system to the hardening of the mth slip system.

It can be seen that there exist saturated values d_1 and $1 + \sum_{k \neq m} f_{mk}$ for f_m and H_m, respectively. It is easily shown that there exists a saturated value for the shear stress on a slip system when plastic deformation fully develops, and the hardening modulus T_m tends to vanish as the shear stress tends to this saturated value.

4. Application and verification

4.1. Incremental form of the proposed constitutive relation

It has been pointed out by PENG and FAN [20] that when α is very large, rewriting Eq. (2.6) directly in an incremental form will induce a very large error in numerical analysis and even affect the convergence of the solution. To avoid this situation, the integral of Eq. (2.6) is introduced and the following incremental constitutive equation is derived [20]:

$$\Delta\tau^{(m)} = A_m \Delta\gamma^{(m)} + B_m \Delta z^{(m)} \quad (m \text{ not summed}), \tag{4.1}$$

in which

$$A_m = k_m C, \qquad B_m = -k_m \alpha \tau^{(m)}(z_n^{(m)}), \quad z^{(m)} = z_n^{(m)} + \Delta z^{(m)} \quad (m \text{ not summed}), \tag{4.2}$$

$$k_m = \frac{1 - e^{-\alpha \Delta z^{(m)}}}{\alpha \Delta z^{(m)}}, \quad \Delta z^{(m)} = \frac{\Delta\zeta^{(m)}}{f_m H_m}, \qquad \Delta\zeta^{(m)} = \left|\Delta\gamma^{(m)}\right|$$

$z_n^{(m)}$ and $\tau^{(m)}(z_n^{(m)})$ denote respectively the generalized time scale and the shear stress of the mth slip system after nth incremental loading, with which Eq. (2.8) can be expressed as

$$\Delta\tau^{(m)} = T_m \Delta\gamma^{(m)}, \quad T_m = A_m + \frac{\Gamma_m B_m}{f_m H_m}, \quad \Gamma_m = \frac{\Delta\gamma^{(m)}}{\Delta\zeta^{(m)}} \quad (m \text{ not summed}). \tag{4.3}$$

The constitutive relation for a single crystal can then be expressed in the following incremental form

$$\Delta\tau^{(m)} = \sum_{n=1}^{N} h_{mn} \Delta\gamma^{(n)}. \tag{4.4}$$

4.2. Polycrystalline analysis based on KBW's self-consistent theory

Suppose the considered crystals and polycrystals are plastically incompressible, in the case of isothermal and small deformation, KBW's self-consistent model gives [5, 21]

$$\Delta\sigma_c - \Delta\overline{\sigma} = -2G(1-\beta)(\Delta\varepsilon_c^p - \Delta\overline{\varepsilon}^p), \tag{4.5}$$

where $\Delta\sigma_c$ and $\Delta\varepsilon_c^p$ denote respectively the increments of stress and plastic strain in a single crystal, $\Delta\overline{\sigma}$ and $\Delta\overline{\varepsilon}^p$ the increments of averaging stress and plastic strain of the polycrystal, G elastic shear modulus of the material, and β satisfies

$$2G(1-\beta) = \frac{2(7-5v)}{15(1-v)}G, \tag{4.6}$$

in which v denotes Poisson's ratio. It is easily obtained from Eq. (4.5) that

$$(\Delta\sigma_c)_{kk} = \Delta\overline{\sigma}_{kk}, \qquad \Delta\mathbf{s}_c - \Delta\overline{\mathbf{s}} = -2G(\Delta\varepsilon_c^p - \Delta\overline{\varepsilon}_c^p - \Delta\overline{\varepsilon}^p), \tag{4.7}$$

where $\Delta\mathbf{s}_c$ and $\Delta\overline{\mathbf{s}}$ are, respectively, the incremental deviatoric stresses of single crystal and polycrystal, respectively. By defining $\Delta\mathbf{q}$ as follows

$$\Delta\mathbf{q} = \Delta\overline{\mathbf{s}} + \frac{2(7-5v)}{15(1-v)}G\Delta\overline{\varepsilon}^p = \Delta\mathbf{s}_c + \frac{2(7-5v)}{15(1-v)}G\Delta\varepsilon_c^p \tag{4.8}$$

and using

$$\Delta\varepsilon_c^p = \sum_{m=1}^{N} \boldsymbol{\alpha}^m \Delta\gamma^{(m)}, \qquad \Delta\tau^{(m)} = \boldsymbol{\alpha}^{(m)} : \Delta\mathbf{s}_c, \tag{4.9}$$

one obtains

$$\sum_{m=1}^{N} A_{nm}\Delta\gamma^{(m)} = b_n, \qquad (n = 1, 2, ..., N), \tag{4.10}$$

in which

$$A_{nm} = h_{nm} + \frac{2(7-5v)}{15(1-v)}G\boldsymbol{\alpha}^{(n)} : \boldsymbol{\alpha}^{(m)}, \qquad b_n = \Delta\mathbf{q} : \boldsymbol{\alpha}^{(n)}. \tag{4.11}$$

In the above equations the macroscopic plastic strain increment $\Delta\overline{\varepsilon}^p$ is related to the plastic strain increment of each crystal $\Delta\varepsilon_c^p$ by a certain averaging procedure, i.e.,

$$\Delta\overline{\varepsilon}^p = \{\Delta\varepsilon_c^p\} \tag{4.12}$$

and the increment of stress can then be calculated by

$$\Delta\overline{\mathbf{s}} = 2G\,(\Delta\overline{\mathbf{e}} - \Delta\overline{\boldsymbol{\varepsilon}}^{p})\,, \qquad \Delta\overline{\sigma}_{kk} = 3K\Delta\overline{\varepsilon}_{kk}, \tag{4.13}$$

in which $\Delta\overline{\mathbf{e}}$ is the deviatoric strain increment of the material, and K is the elastic volumetric modulus.

4.3 Averaging procedure

In general, Eq. (4.12) can be specified as follows

$$\Delta\overline{\boldsymbol{\varepsilon}}^{p} = \frac{1}{V}\sum_{i=1}^{N}\Delta\boldsymbol{\varepsilon}_{c}^{p(i)}V_i \tag{4.14}$$

in which $\Delta\boldsymbol{\varepsilon}_{c}^{p(i)}$ and V_i represent respectively the plastic strain increment and the volume of the ith single crystal, and V is the volume of the polycrystal. If one further assumes that the volume of crystals are identical, i.e., $V = N'V_i$, then Eq. (4.14) can be rewritten as

$$\Delta\overline{\boldsymbol{\varepsilon}}^{p} = \frac{1}{N'}\sum_{i=1}^{N'}\Delta\boldsymbol{\varepsilon}_{c}^{p(i)}. \tag{4.15}$$

In analysis, polycrystal is usually considered as an aggregate of numerous single crystals with randomly distributed orientations. With this assumption, Eq. (4.15) can be expressed as an integral and then calculated with Gaussian quadrature approach [22]. This method, in substance, determines approximately the response of a polycrystal through the single crystals with some specific orientations by weight factors, and can hardly guarantee that the chosen orientations are spatially uniformly distributed, especially in the directions of θ and ϕ (see Fig. 2). To overcome this shortcoming, a mixed averaging approach is used in polycrystalline analysis, which is based on an icosahedron: the outer normal directions of the 20 faces determine 20 spatially uniformly distributed orientations and are represented by 20 sets of θ_i and ϕ_i $(i = 1, 2, ..., 20)$, and in each face it is assumed that there are numerous single crystals with randomly distributed orientations, i.e., ω varies continuously (see Fig. 2). If the arithmetic averaging procedure is used for θ_i and ϕ_i $(i = 1, 2, ..., 20)$ and integral averaging for ω, Eq. (4.15) can be rewritten as

$$\Delta\overline{\boldsymbol{\varepsilon}}^{p} = \frac{1}{20}\sum_{i=1}^{20}\frac{1}{2\pi}\int_{0}^{2\pi}\Delta\boldsymbol{\varepsilon}_{c}^{p}(\theta_i, \phi_i, \omega)d\omega. \tag{4.16}$$

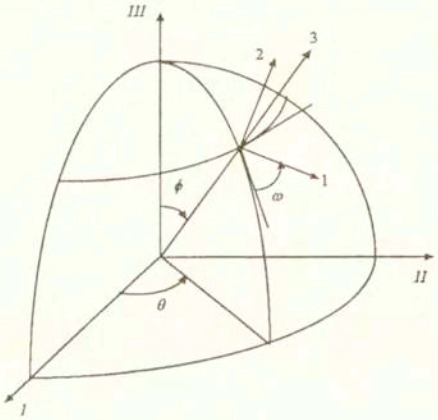

FIG. 2. Global and local coordinate systems.

It is found that: (1) the 20 faces of an icosahedron can be separated into 10 sets, in each of which the two faces are parallel to each other; and (2) the integral range of ω can be reduced to $[0, \pi/2]$ due to symmetry. The above equation can, therefore, be rewritten as

$$\Delta\overline{\varepsilon}^p = \frac{1}{10}\sum_{i=1}^{10}\frac{2}{\pi}\int_0^{\frac{\pi}{2}}\Delta\varepsilon_c^p(\theta_i,\phi_i,\omega)d\omega. \tag{4.17}$$

Further applying the Gaussian quadrature to Eq. (4.17), one obtains

$$\Delta\overline{\varepsilon}^p = \frac{1}{20}\sum_{i=1}^{10}\sum_{j=1}^{4}A_j^{\omega}\Delta\varepsilon_c^p(\theta_i,\phi_i,\omega_j), \tag{4.18}$$

where the coordinates of the Gaussian integration points ω_j and the corresponding weighted coefficients A_j^{ω} are listed in Table 1 (see Appendix), and the values of the 10 sets of independent θ_i and $\phi_i (i = 1, 2, ..., 10)$ are listed in Table 2.

The above averaging procedure involves the response of 40 single crystals with different orientations even if the improvement by the Gaussian weighed coefficients is not considered. It should be stressed that the distribution of the orientations determined by the chosen θ_i and ϕ_i are spatially uniform.

Table 1. The coordinates of Gaussian points ω_j and the corresponding weighted coefficients A_j^{ω}.

j	1	2	3	4
ω_j (rad)	0.1090633	0.5183777	1.052419	1.461733
A_j^{ω}	0.3478548	0.6521452	0.6521452	0.3478548

Table 2. Values of the independent 10 sets of θ_i and ϕ_i.

j	1	2	3	4	5	6	7	8	9	10
$\theta_j(^\circ)$	0	72	144	216	288	288	216	144	72	0
$\phi_j(^\circ)$	37.38	37.38	37.38	37.38	37.38	142.62	142.62	142.62	142.62	142.62

4.4. Application and verification

The cyclic plasticity of 316 stainless steel subjected to some typical biaxial nonproportional plastic strain paths is analyzed. The material has a face-centered-cubic (FCC) crystal lattice. In the local coordinate systems the **n** and **s** of the 12 independent slip systems are listed sequentially in Table 3.

Table 3. 12 sets of independent n and s of FCC crystal.

	1	2	3	4	5	6	7	8	9	10	11	12
n	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}\,\bar{1})$	$(1\bar{1}\,\bar{1})$	$(1\bar{1}\,\bar{1})$	(111)	(111)	(111)
s	[101]	[011]	$[1\bar{1}0]$	[110]	[011]	$[10\bar{1}]$	[101]	[110]	$[01\bar{1}]$	$[10\bar{1}]$	$[0\bar{1}1]$	$[1\bar{1}0]$

Following BASSANI'S consideration [10], the coupled hardening coefficients f_{mn} can be expressed in the form of a matrix as follows in terms of the sequence of the independent slip systems (see Table 3)

$$[f_{mn}] = \begin{bmatrix} 0 & C_1 & C_1 & C_3 & C_2 & C_1 & C_1 & C_2 & C_2 & C_1 & C_3 & C_2 \\ & 0 & C_1 & C_2 & C_1 & C_2 & C_1 & C_3 & C_1 & C_3 & C_1 & C_2 \\ & & 0 & C_1 & C_2 & C_3 & C_2 & C_1 & C_3 & C_2 & C_2 & C_1 \\ & & & 0 & C_1 & C_1 & C_2 & C_1 & C_2 & C_2 & C_3 & C_1 \\ & & & & 0 & C_1 & C_3 & C_2 & C_1 & C_2 & C_1 & C_3 \\ & & & & & 0 & C_1 & C_2 & C_3 & C_1 & C_2 & C_2 \\ & & & & & & 0 & C_1 & C_1 & C_1 & C_2 & C_3 \\ & & & & & & & 0 & C_1 & C_3 & C_2 & C_1 \\ & & & & & & & & 0 & C_2 & C_1 & C_2 \\ & & & \text{sym.} & & & & & & 0 & C_1 & C_1 \\ & & & & & & & & & & 0 & C_1 \\ & & & & & & & & & & & 0 \end{bmatrix}$$

A procedure for the analysis of the stress (or strain) response of polycrystalline materials subjected to a strain (or stress) history was suggested by PENG *et al.* [23], where no additional iteration is used for the determination of the activation of slip systems and the direction of slip. It greatly simplifies the numerical process. The stress response of 316 stainless steel subjected to nonproportional strain cycling was analyzed and experimentally verified [23].

When deformation is controlled by plastic strain, the numerical process becomes more complicated. The macroscopic stress increment $\Delta\bar{\mathbf{s}}$ and the stress increment $\Delta\mathbf{s}_c$ of each crystal can not be known before the shear stress of each slip system, $\Delta\tau^{(m)}$, is obtained, so that $\Delta\mathbf{s}_c$ has to be determined by solving the following equation:

$$\boldsymbol{\alpha}^{(m)} : \Delta\mathbf{s}_c = \Delta\tau^{(m)} \qquad (m = 1, 2, ..., N). \tag{4.19}$$

There are 12 equations in Eq. (4.18) for FCC crystal and it can be shown that there are five independent ones among them. It should be emphasized that in the framework of the employed constitutive model, no yield criterion is used and the relation between slip and the corresponding shear stress is smooth and continuous. Slip occurs at extremely low rate at the onset of loading and unloading but increases and speeds up as $\tau^{(m)}$ increases. At any stage of deformation, $\Delta\tau^{(m)}$ can uniquely be determined by the given $\Delta\gamma^{(m)}$ (see Eq. (4.4)), and inversely, $\Delta\gamma^{(m)}$ can also be uniquely determined by the given $\Delta\tau^{(m)}$. This feature greatly simplifies the numerical process, in which one can simply select and fix five independent slip systems *a priori* without considering if slip occurs on each system or not. Given a set of $\Delta\tau^{(m)}$, the five components of the corresponding $\Delta\mathbf{s}_c$ can be obtained by solving Eq. (4.19). The increment of the polycrystalline stress $\Delta\bar{\mathbf{s}}$ is then related to $\Delta\mathbf{s}_c$ of each crystal by some averaging procedure, i.e.,

$$\Delta\bar{\mathbf{s}} = \{\Delta\mathbf{s}_c\}. \tag{4.20}$$

The following averaging procedure similar to Eq. (4.17) can be derived from Eqs. (4.7), (4.12) and (4.18)

$$\Delta\bar{\mathbf{s}} = \frac{1}{20}\sum_{i=1}^{10}\sum_{j=1}^{4} A_j^{\omega}\,\Delta\mathbf{s}_c(\theta_i, \phi_i, \omega_j). \tag{4.21}$$

In the conventional theory of crystal plasticity, no slip occurs in a slip system if the shear stress is less than the critical shear stress. In other words, the relation between stress and slip is not unique before slip occurs. When solving $\Delta\mathbf{s}_c$ from Eq. (4.19), one can hardly select and fix 5 independent equations from the 12 ones *a priori*. For nonproportional loading, searching for this kind of 5 independent equations is tedious and needs some additional principle such as the

principle of maximum plastic work proposed by BISHOP and HILL [24] to reduce the computational difficulty.

A numerical procedure for the analysis of the elastoplastic behavior of a polycrystalline material subjected to nonproportional plastic strain histories is proposed as follows: with the result obtained in the kth iteration of the nth increment of loading, such as $\Delta\bar{\mathbf{s}}_{(n)}^{(k)}$ of the material, $\Delta\boldsymbol{\varepsilon}_{c(n)}^{p(k)}$ and $\Delta\mathbf{s}_{c(n)}^{(k)}$ of each single crystal and $\{\Delta\gamma^{(m)}\}_{(n)}^{(k)}$, $\{\Delta\zeta^{(m)}\}_{(n)}^{(k)}$, $\{\Delta z^{(m)}\}_{(n)}^{(k)}$ of each slip system, one can calculate $[h_{ij}]_{(n)}^{(k)}$ with Eqs. (4.2), (4.3) and (2.10). Given an increment of plastic strain $\Delta\boldsymbol{\varepsilon}_{(n)}^{p}$, $\Delta\mathbf{q}_{(n)}^{(k+1)}$ can be calculated with Eq. (4.8) and then $[A_{ij}]_{(n)}^{(k)}$, $\{b_j\}_{(n)}^{(k)}$ with Eq. (4.11), $\{\Delta\gamma^{(m)}\}_{(n)}^{(k+1)}$ by solving Eq. (4.10) and $\{\Delta\tau^{(m)}\}_{(n)}^{(k+1)}$ by Eq. (4.4). $\Delta\mathbf{s}_{c(n)}^{(k+1)}$ of each crystal can be obtained by solving Eq. (4.19) and $\Delta\bar{\mathbf{s}}_{(n)}^{(k+1)}$ by Eq. (4.21). The iterative process continues until the following inequality is satisfied

$$\delta = \max_{j=1}^{N'} \frac{||\Delta\mathbf{q}_{(n)}^{(k+1)} - \Delta\mathbf{q}_{(n)}^{(k)}||}{||\Delta\mathbf{q}_{(n)}^{(k+1)}||} \leq \delta_0, \tag{4.22}$$

where N' is the total number of the single crystals used in the calculation, δ and δ_0 are respectively the maximum relative error and the tolerant error. The value of δ_0 is chosen as 1% in the calculation. Then the obtained incremental results are added respectively to the corresponding results up to the $(n-1)$th increment of loading and one, therefore, obtains $\mathbf{s}_{(n)}$ of the polycrystalline material, $\{\boldsymbol{\varepsilon}_c^p\}_{(n)}$ of each single crystal, $\{\tau^{(m)}\}_{(n)}$, $\{\zeta^{(m)}\}_{(n)}$, $\{z^{(m)}\}_{(n)}$, $\{f_m\}_{(n)}$, $\{H_m\}_{(n)}$ of each slip system, and starts the calculation of the next increment of loading.

The response of 316 stainless steel subjected to biaxial nonproportional plastic strain cycling at room temperature is analyzed with the proposed approach. The material is considered as an aggregate of single crystals with FCC lattice structure. The material constants are determined as follows from the experimental result [11]:

$$G = 78 \text{ GPa}, \quad \nu = 0.23,$$

$$C = 2.92 * 10^3 \text{ GPa}, \quad \alpha = 3.2 * 10^4, \quad d_c = 1.0,$$

$$C_1 = 0.04, \quad C_2 = 0.30, \quad C_3 = 0.50, \quad \beta_s = 15.$$

The constitutive behavior of a slip system during loading-unloading and reloading determined by the constitutive model is shown in Fig. 3 without taking into account the cross-hardening. The solid line corresponds to the determined C, α and d_c; while the dashed line corresponds to the same d_c but both C and α are reduced to 10 percent of the determined values. It is seen that when α is

sufficiently large, the constitutive behavior of a slip system is quite close to that using the slip model containing a yield criterion, and an appropriate choice of α can describe to some extent the Bauschinger effect. For biaxial analysis, we define the following stress and strain vectors:

$$\vec{\sigma} = \sigma \mathbf{n}_1 + \sqrt{3}\tau \mathbf{n}_2, \qquad \vec{\varepsilon}^p = \varepsilon^p \mathbf{n}_1 + \frac{1}{\sqrt{3}}\gamma^p \mathbf{n}_2 \tag{4.23}$$

in which σ and τ denote the tensile and shear stress, respectively, ε^p and γ^p the tensile and shear plastic strain, $\mathbf{n}_1$ and $\mathbf{n}_2$ are two unit vectors perpendicular to each other. We also define the equivalent stress, equivalent plastic strain and the accumulative plastic strain as follows:

$$\sigma_e = |\vec{\sigma}| = \sqrt{\sigma^2 + 3\tau^3}, \qquad \varepsilon_e^p = |\vec{\varepsilon}^p| = \sqrt{(\varepsilon^p)^2 + \frac{1}{3}(\gamma^p)^2}, \tag{4.24}$$

$$\zeta^p = \int |d\vec{\varepsilon}^p|.$$

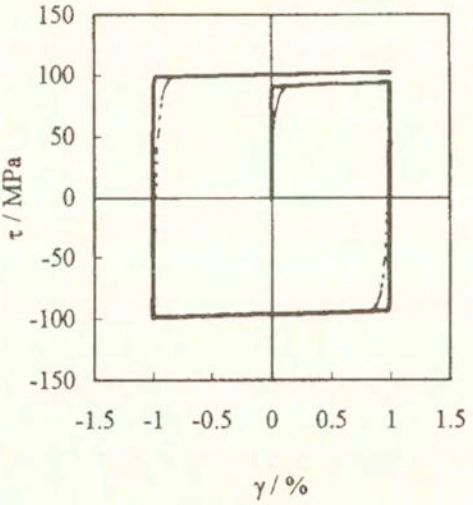

FIG. 3. The loading-unloading and reloading behavior of a slip system without considering cross-hardening.

The calculated $\sigma - \varepsilon^p$ curve of the material subjected to symmetrically tensile-compressive plastic strain cycling with a fixed equivalent plastic strain amplitude $\varepsilon_a^p = 0.2\%$ is shown in Fig. 4. And the relation between $\sqrt{3}\tau$ and $\frac{1}{\sqrt{3}}\gamma^p$ of the material subjected to symmetrically plastic shear strain cycling with the same equivalent plastic strain amplitude is shown in Fig. 5. Both are in satisfactory agreement with the experimental result [11]. It is seen by comparing Fig. 4 with

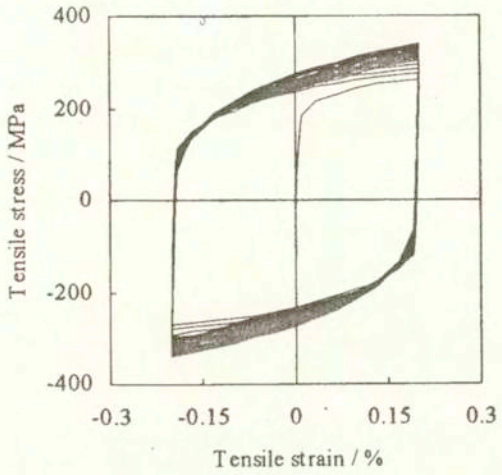

FIG. 4. Calculated $\sigma - \varepsilon^p$ curve corresponding to symmetrically tensile-compressive plastic strain cycling with $\varepsilon_a^p = 0.2\%$.

Fig. 5 that besides the minor difference between the hysteresis loops, the calculated equivalent stress amplitude corresponding to plastic shear strain cycling are distinctly less than that corresponding to tensile-compressive plastic strain cycling (also see Fig. 8) although the equivalent plastic strain amplitudes are identical. This phenomenon also coincides with the experimental observation and can mainly be attributed to the difference of the activation of slip systems under these two kinds of loading conditions, which can not be well described by simply using the Mises equivalent rule.

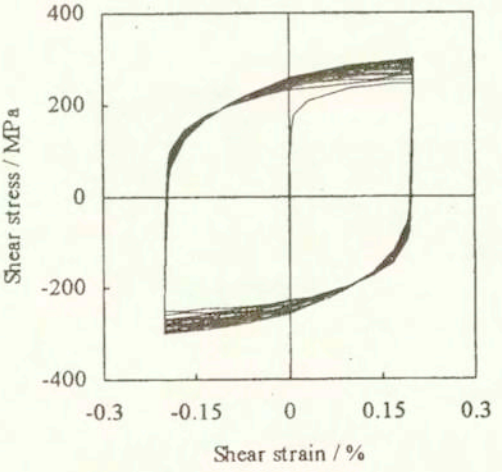

FIG. 5. Calculated $\sqrt{3}\tau - \gamma^p/\sqrt{3}$ curve corresponding to symmetrically plastic shear strain cycling with $\gamma_a^p/\sqrt{3} = 0.2\%$.

In the analysis of the response of materials subjected to nonproportional plastic strain cycling, one usually defines the radius of the minimal super-sphere surrounding the cyclic plastic strain path as equivalent plastic strain amplitude ε_a^p. Figure 6(a) and (b) show respectively the calculated and experimental [11] biaxial stress trajectories corresponding to the square path with $\varepsilon_a^p = 0.2\%$ in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane (the coordinates of the four corners are $(0.2\%, 0)$, $(0, 0.2\%)$, $(-0.2\%, 0)$ and $(0, -0.2\%)$, sequentially), and Fig. 7(a) and (b) the calculated and experimental [11] stress trajectories corresponding to the 90° out-of-phase

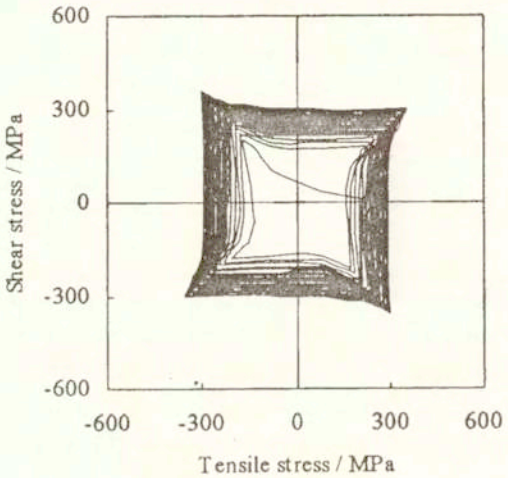

FIG. 6. a) Calculated stress trajectory in $\sigma - \sqrt{3}\tau$ plane corresponding to the cyclic square path in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane.

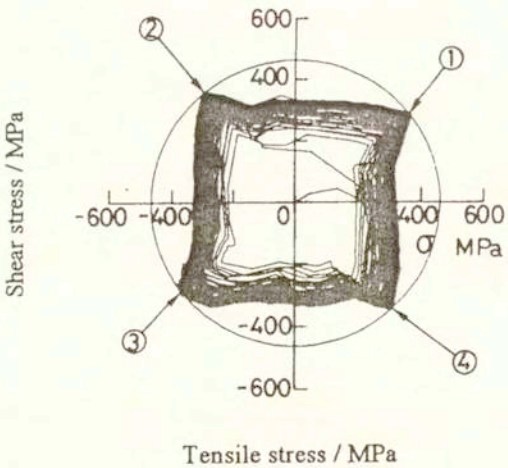

FIG. 6. b) Experimental stress trajectory in $\sigma - \sqrt{3}\tau$ plane corresponding to the cyclic square path in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane.

(circular) path with $\varepsilon_a^p = 0.2\%$, respectively. The comparison between the calculated and experimental results shows reasonable agreement. Compared with the results corresponding to the proportional paths (see Figs. 4 and 5), the stress amplitudes in Figs. 6 and 7 increase about 50% (see Fig. 8). This marked difference can be attributed to the cross-hardening caused by the intersection between the moving dislocations and the dislocation forests, the dislocation tangle and

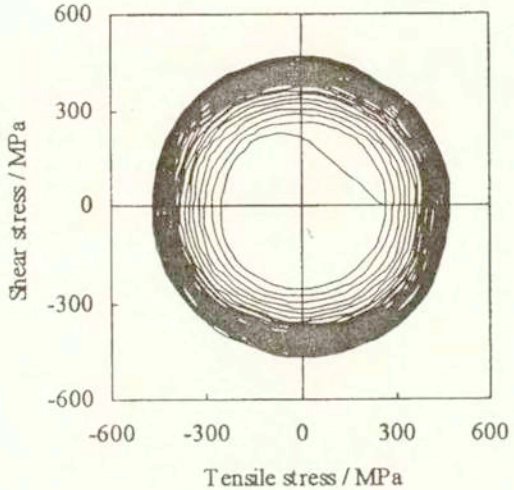

FIG. 7. a) Calculated stress trajectory in $\sigma - \sqrt{3}\tau$ plane corresponding to the cyclic circular path in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane.

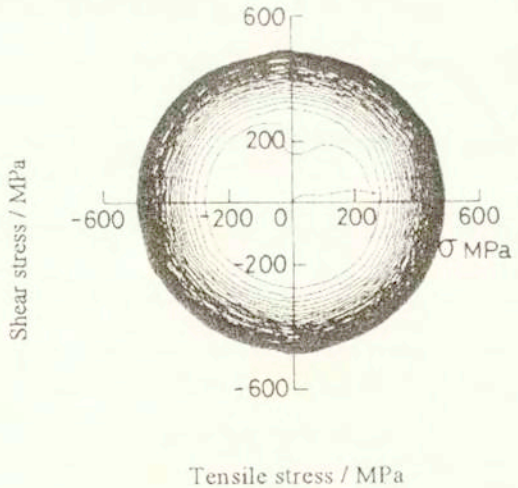

FIG. 7. b) Experimental stress trajectory in $\sigma - \sqrt{3}\tau$ plane corresponding to the cyclic circular path in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane.

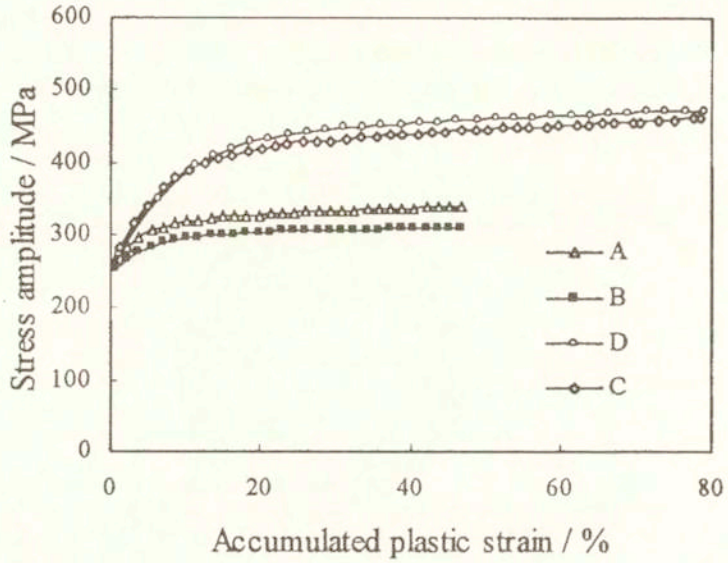

FIG. 8. a) Calculated relation between equivalent stress amplitudes and accumulated plastic strain along different plastic strain paths.

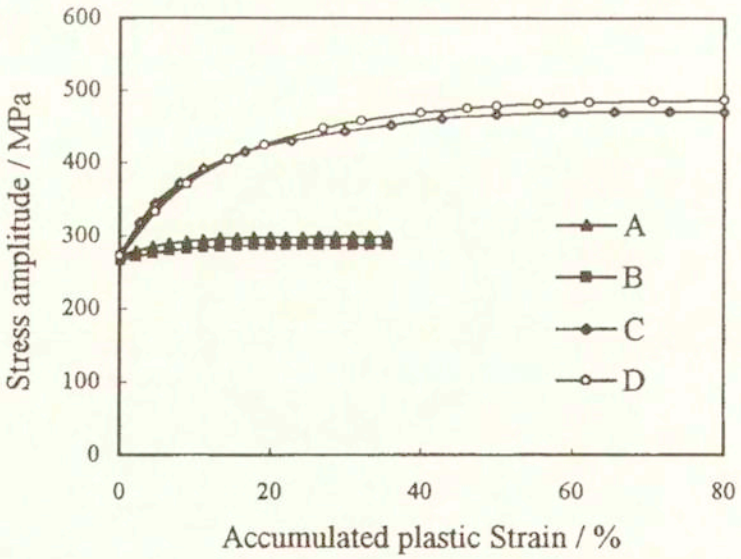

FIG. 8. b) Experimental relation between equivalent stress amplitudes and accumulated plastic strain along different plastic strain paths.

the corresponding substructures induced by which may greatly increase the resistance to dislocation glide. In phenomenological analysis, such kind of increase is usually attributed to the nonproportionality of the plastic strain path and is considered by introducing an appropriate measure of nonproportionality and the corresponding hardening laws [13, 23, 25]. In the proposed approach, the response is satisfactorily described by considering the interaction of dislocations along different slip systems. The variation of the equivalent stress amplitude σ_a against the accumulative plastic strain ζ^p along the above four typical paths in $\varepsilon^p - \gamma^p/\sqrt{3}$ plane with a constant strain amplitude $\varepsilon_a^p = 0.2\%$ is shown in Fig. 8. These plastic strain paths can be classified to proportional ones (cyclic tension-compression and cyclic torsion, respectively) and nonproportional ones (square path and circular path). Calculation shows that, for the proportional plastic strain cycling the equivalent stress amplitudes are relatively small, but for the cycling along nonproportional plastic strain paths, the equivalent stress amplitudes greatly increase. The qualitative and quantitative agreement between the calculated and experimental results [11] demonstrates the validity of the proposed approach in the analysis of plastic strain controlled nonproportional cyclic crystalline plasticity.

5. Discussion and conclusion

During inelastic deformation process, a part of energy can be stored in the substructure of materials in the form of residual microstress fields and this part of energy can be released under some condition so that the external energy to activate and motivate dislocations can be reduced. With this viewpoint, a constitutive relation for a slip system is derived based on a simple mechanical model consisting of a spring and a plastic dashpot-like block. The corresponding hardening law for single crystal and the approach based on KBW's self-consistent theory for polycrystalline analysis is then obtained. The constitutive model contains no yield criterion and the corresponding numerical analysis is greatly simplified.

A mixed averaging approach is used to analyze the response of polycrystalline materials. It is based on 20 sets of θ_i and ϕ_i representing 20 spatially uniformly distributed orientations, and in each face with a set of θ_i and ϕ_i as its normal it is assumed that there are numerous single crystals with randomly distributed orientations. An arithmetic averaging procedure is used for θ_i and $\phi_i (i = 1, 2, ..., 20)$ and Gaussian quadrature averaging procedure is used for ω.

A valuable discussion on the crystal orientation distribution was given in [26], in which the volume of FCC crystal orientation space was shown and the minimal size of the orientation regions for crystals was suggested. In the present analysis, it seems from Eq. (4.17), Tables 1 and 2 that the orientation region for crystals is

$(0 \leq \theta < 2\pi, 0 \leq \phi < \pi/2, 0 \leq \omega < \pi/2)$. The values of θ used in the analysis are $(0°, 72°, 144°, 216°, 288°)$. Calculation shows that if the values of θ were replaced by $(0°, 72°, 144°, 36°, 108°)$, i.e., the region of θ was reduced to $[0, \pi)$, identical results for all the given plastic strain paths would be obtained. But if they were further replaced by $(0°, 72°, 54°, 36°, 18°)$, i.e., the region of θ was reduced to $[0, \pi/2)$, a marked difference was detected. It indicates that the adopted orientation region for crystals may further reduce to $(0 \leq \theta < \pi, 0 \leq \phi < \pi/2, 0 \leq \omega < \pi/2)$ and a conservative estimation for the volume of the orientation space is

$$\Omega = \int_0^{\pi} d\theta \int_0^{\frac{\pi}{2}} d\omega \int_0^{\frac{\pi}{2}} \sin\phi d\phi = \frac{\pi^2}{2},$$

which is a little larger than the volume of FCC crystal orientation space [26] and may result in some equivalent orientations when the number of the used orientations is large.

The cyclic plasticity of 316 stainless steel subjected to four typical biaxial nonproportional plastic strain paths was analyzed and experimentally verified. Calculation also showed that the corresponding numerical algorithm is of good convergence and efficiency.

Appendix

Gaussian quadrature can be expressed as

$$\int_{-1}^{1} f(x)dx = \sum_{k=1}^{n} A_k f(x_k). \tag{A.1}$$

Suppose the orientation region for crystals is $(a_1 \leq \theta < a_2, b_1 \leq \phi < b_2, c_1 \leq \omega < c_2)$, the averaging of s is given as

$$< \mathbf{s} >= \frac{1}{\Omega} \int_{a_1}^{a_2} d\theta \int_{c_1}^{c_2} d\omega \int_{b_1}^{b_2} \mathbf{s}(\theta, \phi, \omega) \sin\varphi d\varphi, \tag{A.2}$$

where

$$\Omega = \int_{a_1}^{a_2} d\theta \int_{c_1}^{c_2} d\omega \int_{b_1}^{b_2} \sin\phi d\phi. \tag{A.3}$$

If the θ, ω and ϕ are replaced respectively with $\frac{1}{2}[(a_2 - a_1)x + (a_2 + a_1)]$, $\frac{1}{2}[(c_2 - c_1)y + (c_2 + c_1)]$, and $\arccos\left\{\frac{1}{2}[(\cos b_1 - \cos b_2)z + (\cos b_1 + \cos b_2)]\right\}$, Eq. (A.2) can be rewritten as follows by using Eq. (A.3)

$$< \mathbf{s} >= \frac{1}{8}\int_{-1}^{1} dx \int_{-1}^{1} dy \int_{-1}^{1} \mathbf{s} dz, \tag{A.4}$$

where

$$\mathbf{s} = \mathbf{s}\left(\frac{1}{2}[(a_2 - a_1)x + (a_2 + a_1)], \quad \frac{1}{2}[(c_2 - c_1)y + (c_2 + c_1)], \right.$$
$$\left. \arccos\left\{\frac{1}{2}[(\cos b_1 - \cos b_2)z + (\cos b_1 + \cos b_2)]\right\}\right).$$

Eq. (A.4) can then be numerically calculated by

$$< \mathbf{s} >= \frac{1}{8}\sum_{i=1}^{N_i}\sum_{j=1}^{N_j}\sum_{k=1}^{N_k} A_i^{\theta} A_j^{\omega} A_k^{\varphi} \mathbf{s}(\theta_i, \omega_j \phi_k), \tag{A.5}$$

where N_i, N_j, N_k and A_i^{θ}, A_j^{ω}, A_k^{φ} denote the number of integration points and the weight coefficients.

If the orientation region consists of n subregions $\Omega_i (I = 1, ..., n)$, the averaging of s can be calculated with

$$< \mathbf{s} >= \frac{1}{\Omega}\sum_{i=1}^{n}\int_{\Omega_i} \mathbf{s} d\Omega = \sum_{i=1}^{n}\frac{\Omega_i}{\Omega}\frac{1}{\Omega_i}\int_{\Omega_i} \mathbf{s} d\Omega = \sum_{i=1}^{n} V_i < \mathbf{s} >_i \tag{A.6}$$

in which V_i and $< \mathbf{s} >_i$ denote respectively the volume fraction and the averaging of s of the ith subregion.

At the given range of orientation region for crystals and the number of Gaussian integration points, one can find the coordinates of the integration points and the corresponding weight coefficients. For example, for $0 \leq \omega < \pi/2$, and using four integral points, one can find that the coordinates of the Gaussian integration points are $y_{1,2} = \pm 0.3399810$ and $y_{3,4} = \pm 0.8611363$, which corresponds to $\omega_{1,2,3,4} = 0.5183777$, 1.052419, 0.1090633, 1.461733 (rad), the corresponding weight coefficients are $A_1^{\omega} = A_2^{\omega} = 0.6521452$ and $A_3^{\omega} = A_4^{\omega} = 0.3478548$ which are the values given in Table 1.

Acknowledgment

Financuially supported by WSFC and the Education Ministry of China.

References

1. G. I. TAYLOR, *Plastic strain in metals*, J. Inst. Metals, **62**, 307–324, 1938.
2. R. HILL, *Generalized constitutive relations for incremental deformation of metals and crystals multislip*, J. Mech. Phys. Solids, **14**, 95–102, 1966.
3. R. HILL and J.R. RICE, *Constitutive analysis of elastic-plastic crystals at arbitrary strain*, J. Mech. Phys. Solids, **20**, 401–413, 1972.
4. E. SCHMID and W. BOAS, *Kristallplastizität*, Springer-Verlag, Berlin 1950.
5. B. BUDIANSKY and T.T. WU, *Theoretical prediction of plastic strain of polycrystals*, Proc 4th US national Congr. Appl. Mech., 1175–1185, 1962.
6. J. W. HUTCHINSON, *Elastic-plastic behavior of polycrystalline metals and composites*, Proc Roy Soc London, A., **319**, 247–272, 1970.
7. G. J. WENG, *Kinematic hardening rule in single crystals*, Int. J. Solids & Struct., **15**, 861–875, 1979.
8. G. J. WENG, *Dislocation theories of work hardening and yield surfaces of single crystals*, Acta Mech., **37**, 217–228, 1980.
9. R. J. ASARO, *Crystal plasticity*, J. Appl. Mech., **50**, 921–934, 1983.
10. J. L. BASSANI, *Single crystal hardening*, Appl. Mech. Rev., **43**(5), 320–327, 1990.
11. E. TANAKA, S. MURAKAMI and M. OOKA, *Effect of strain path shape on nonproportional cyclic plasticity*, J. Mech. Phys. Solids, **33**, 559–575, 1985.
12. Z. R. SONG, *The physics of metals*, Vol II, High Education Press, Beijing 1992.
13. J. FAN and X. PENG, *A physically based constitutive description for nonproportional cyclic plasticity*, J. Engng. Mat. Tech., **113**, 254–262, 1991.
14. X. PENG and A.R.S. PONTER, *A constitutive law for two-phase materials with experimental verification*, Int. J. Solids & Struct., **31**, 8, 1099–1111, 1994.
15. X. PENG, C. MEYER and L. FANG, *A thermomechanically consistent continuum damage model for concrete meterials*, ASCE, J. Engng. Mech., **123**, 1, 60–69, 1997.
16. K. C. VALANIS, *Fundamental consequences of new intrinsic time measure plasticity as a limit of the endochronic theory*, Arch. Mech., **23**, 171–190, 1980.
17. J. L. CHABOCHE and G. ROUSSELIER, *On plastic and viscoplastic constitutive equations*, J. Pressure Vessel Tach., **105**, 153–164, 1983.
18. H. MURAKAMI and H.E. READ, *Endochronic plasticity: some basic properties of plastic flow and failure*, Int. J. Solids & Struct., **23**, 133–151, 1987.
19. W. KOITER, *Stress-strain relation, uniqueness and variational theorems for elastic-plastic materials with singular yield surface*, Quert. Appl. Math., **11**, 350–359, 1953.
20. X. PENG and J. FAN, *A new numerical approach for nonclassical plasticity*, Computers and Structures, **47**, 2, 313–320, 1993.
21. E. KRÖNER, *Zur plastichen verformung des vielkristalls*, Acta Metall., **9**, 155–165, 1961.

22. K. HWANG and S. SUN, *Micromechanical modeling of cyclic plasticity*, Advances in Engineering Plasticity: 41–48, Proc. Second Asia-Pacific Symposium on Advances in Engineering Plasticity and Its Applications, Edited by B Xu and W Yang, International Academic Publishers, Beijing 1994.

23. X. PENG, X. ZENG and J. FAN, *On a nonclassical constitutive theory of crystal plasticity*, Mechanics Research Communication, **24**, 6, 631–638, 1997.

24. J. F. W. BISHOP and R. HILL, *A theoretical derivation of the plastic properties of a polycrystalline face centered metal*, Philos. Mag., **42**, 414–427, 1951.

25. A. BENALLEL and D. MARQUIS, *Constitutive equation for nonproportional cyclic plasticity*, J. Engng. Mat. Tech., **109**, 326–336, 1987.

26. P. H. DŁUŻEWSKI, *Crystal orientation spaces and remarks on the modeling of polycrystal anisotropy*, J. Mech. Phys. Solids, **39**, 5, 651–661, 1991.

Received March 10, 1999; new version September 24, 1999.