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◉ 論　文

The investigation of plastic spin behavior of body centered polycrystal with simplified accommodatio model

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정적 결정수용모델에 의한 체심입방격자 다결정의 소성스핀 거동에 관한 연구

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Key Words : Plastic Spin(소성스핀), Finite Deformation(유한변형), Texture(직조), Rate-dependent Plasticity(변형률 의존 소성)

요 약 문

소성스핀을 취급하기 위한 이론을 살펴보면 개념적으로 현저히 다른 세가지로 압축된다. 또한 재료직조 현상이 소성스핀의 근원이라고 알려져 있지만, 그 지배인자와 발생근원에 대해서 아직 충분히 연구되어 있지 않다. 따라서 앞으로의 연구에 올바른 방향을 제시하기 위하여 소성스핀의 기본적인 거동에 대한 연구가 요구된다.

본 연구에서는 체심입방격자 다결정의 소성스핀 시뮬레이션을 통하여, 소성스핀의 거동을 조사하였는데, 재료직조, 변형경화, 변형속도, 하중역전 등의 영향을 검토하였다. 소성발생원인으로 재료직조현상이 강조되었고, 이에 관련한 주요 지배인자를 제시하였다. 무차원 소성스핀은 변형속도, 재료경화에 영향을 받으나 재료직조와 관련한 인자와 비교하여 그 영향이 작게 나타났다.

1. Introduction

Since Kratochvil[1] recognized a need for the constitutive equation of plastic spin, many researches have been studied on this subject. Summarizing them from the conceptual view point, it can be found there are two divergencies.

First, as Kratochvil's statement, an additional constitutive equation has been widely introduced by Loret[2], Dafalias[3,4], Pecherski[5], Zbib and Aifantis[6], Dafalias and Aifants[7], Paulun and

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Pecherski[8], Ning and Aifantis[9], and so on. It has been accepted, in general, that the plastic spin can be described by a function of tensor, which may represent an aspect of internal state of material. Dafalias[3] introduced the isotropic function representation, and proposed the simplest one. The constitutive equation by the representation theory has an unknown coefficient. Paulun and Pecherski[8] treated the coefficient more rationally. Besides the isotropic function approach, Gissen[10,11] proposed a generalized flow rule where a microstress plays an important role in general unsymmetrical tensor.

Second, it was argued by some authors[18,23] that there needs no additional constitutive equation for the plastic spin. According to their works, the additional constitutive equation was made to be a quite redundant one by deriving a kinematic function. Recently Schiek and Stumpf[13] showed the kinematic function consists of purely kinematic quantities with an alternative objective decomposition.

On the other hand, it is interesting that there are quite distinctive concepts each other in the above theories. It can be found that the plastic spin is still an opened subject to be dug out. Therefore, more investigations are needed on the plastic spin to understand its fundamental behavior and to develop its future researches.

The purpose of this paper is to provide a thorough investigation on the plastic spin. The simulation of plastic spin is conducted on a body centered polycrystal using a simple static accommodation model and constitutive equation of Johnston-Gilman type[14]. Based on the present simulation, the effects of texturing, hardening, deformation rate, reverse loading and so on, are investigated. Though the texturing has been known as an origin of plastic spin, its significance is emphasized and the governing factors of the plastic spin are suggested.

2. Simulation model

2.1 Kinematics

Departing from the multiplicative decomposition, as shown in Eq. (2.1) and employing the updated Lagrangian, the deformation gradient tensor F can be evaluated from the reference configuration x^o updated at previous step.

$$F = F^e F^p \tag{2.1}$$

Another reference configuration x^p is related to the configuration x^o by Eq. (2.2).

$$dx^p = F^p dx^o \tag{2.2}$$

The increment of Green strain tensor can be described as follows,

$$\varDelta E = \frac{1}{2}(F^T F - I) = \frac{1}{2}\{(F^p)^T (F^e)^T F^e F^p - (F^p)^T F^p + (F^p)^T F^p - I\} \tag{2.3}$$

where I is an unit diagonal tensor. With the definition of Green strain tensor, Eq. (2.3) is reduced to Eq. (2.4) as follows,

$$\varDelta E = (F^p)^T \varDelta E^e F^p + \varDelta E^p \tag{2.4}$$

where $\varDelta E^e$ is the elastic strain increment measured from x^p and $\varDelta E^p$, the plastic strain increment from x^o.

The velocity gradient of plastic deformation gradient is defined as follows.

$$L^p = \dot{F}^p (F^p)^{-1} \tag{2.5}$$

The plastic deformation gradient is approximately obtained by integrating its velocity gradient and under the assumption of constant velocity gradient during incremental deformation,

$$F^p = e^{(L^t \varDelta t)} \tag{2.6}$$

where Δt is a small time increment. Eq.(2.6) can be evaluated by the characteristic equation theory for a function of matrix. To avoid eigenvalue analysis, Eq.(2.6) is approximated as follow.

$$F^p = I + L^p \Delta t \quad (2.7)$$

From Eq. (2.4), the elastic strain increment can be recast as follows.

$$\Delta E^e = (F^p)^{-T}(\Delta E - \Delta E^p)(F^p)^{-1} \quad (2.8)$$

Finally the plastic velocity gradient L^p is obtained from a constitutive equation, and the plastic spin is defined as follows.

$$W^p = \frac{1}{2}(L^p - (L^p)^T) \quad (2.9)$$

2.2. Formulation of stress increment

The time derivative of Lagrangian tensor is spontaneously objective, namely, Lagrangian objectivity. It is necessary to notice the relation of the Cauchy stress to the second Piola-Kirchhoff stress,

$$\sigma = \frac{1}{J} F \sigma_p (F)^T \quad (2.10)$$

where σ is the Cauchy stress, σ_p the second Piola-Kirchhoff stress, J the determinant of F. Taking time derivative at both sides of Eq.(2.10) and rearranging it, the following objective rate is obtained.

$$\underset{\circ}{\sigma} = \frac{1}{J} F \dot{\sigma}_p (F)^T = \dot{\sigma} - L\sigma - \sigma(L)^T - tr(L)\sigma \quad (2.11)$$

It is well known that the second Piola-Kirchhoff stress is conjugated to the Green strain tensor. The constitutive relation of the second Piola-Kirchhoff stress and Green strain tensor may be given, in incremental form, by

$$\Delta\sigma_p = C : \Delta E^e \quad (2.12)$$

where C is a forth order tensor. By substituting Eq.(2.8) into Eq.(2.12), the following constitutive equation is obtained in terms of total and plastic strain increments,

$$\begin{aligned} \Delta\sigma_p &= C : \{(F^p)^{-T}(\Delta E - \Delta E^p)(F^p)^{-1}\} \\ &= \bar{C} : (\Delta E - \Delta E^p) \end{aligned} \quad (2.13)$$

where $\bar{C} = (F^p)^{-1} C (F^p)^{-T}$ ($\fallingdotseq C$ for small increment).

The updating of stress is approximately performed as follows,

$$\Delta\sigma = \Delta\sigma_p + L\sigma^o \Delta t + \sigma^o (L)^T \Delta t + tr(L)\sigma^o \Delta t \quad (2.14)$$

where σ^o is the Cauchy stress in the configuration x^o.

2.3 Simplified averaging model

Self-consistent models have been suggested to get macroscopic stress and strain from those of grains, but they are cumbersome because many iterations may be needed. Here an approximation will be dared to use instead of rigorous self-consistence performance. A grain stress σ_g is suggested as follows[15].

$$\sigma_g = \sigma + 2\alpha\mu(1-\beta)(e^p - e_g^p) \quad (2.15)$$

By specifying a particular accommodation function α, many accommodation models can be obtained, such as Taylor's, Lin's, Kroner's and static model. Berveiller and Zaoui[15] have shown that the accommodation function is small except at zero macro-plastic strain e^p, and rapidly decreases as the plastic deformation proceeds. Bretheau et al.[16] have suggested further smaller accommodation function in the strain measurement of a grain. From the above context, it is plausible to assume $\sigma_g = \sigma$, namely, static model.

Under the assumption of static model, the plastic deformation gradient is approximated by the following procedure,

$$\begin{aligned} F &= \frac{1}{n_g}\sum_i F_i = \frac{1}{n_g}\sum_i F_i^e F_i^p \\ &= \frac{1}{n_g}\sum_i R^r R_i^* U_i^e F_i^p \end{aligned} \tag{2.16}$$

where F_i is the total deformation gradient of a grain, n_g the number of grains in the aggregate (assumed that all grains have the same volume), R^r the macroscopic rigid body rotation, R_i^* the relative rotation of grain. By $R_i^* U_i^e \doteqdot U_i^e = U^e$ assuming from the static model, the deformation gradient tensor can be decomposed as follows.

$$F = R^r U^e \frac{1}{n_g}\sum_i F_i^p = F^e F^p \tag{2.17}$$

Here it is assumingly confined that only dislocation movements of crystallographic slip systems are responsible for the plastic deformation. Then the plastic velocity gradient is represented by two vectors, gliding direction(s) and normal vector(n) to the slip plane, and slip velocity $\dot{\gamma}$,

$$L^p = \frac{1}{n_g}\left(\sum_{i=1}^{n_g}\sum_{j=1}^{n_s} \dot{\gamma}_{ij} P_{ij}\right) \tag{2.18}$$

where $P_{ij} = s_{ij} \otimes n_{ij}$, the indices (i, j) designate a grain and a slip, respectively (not components of tensor). Substituting Eq.(2.7) into Eq.(2.18), the plastic deformation gradient is expressed as follows.

$$F^p = I + \frac{\Delta t}{n_g}\left(\sum_{i=1}^{n_g}\sum_{j=1}^{n_s} \dot{\gamma}_{ij} P_{ij}\right) \tag{2.19}$$

And the plastic deformation gradient of a grain is, of course, given by the Eq.(2.20).

$$F_i^p = I + \Delta t \sum_{j=1}^{n_s} \dot{\gamma}_{ij} P_{ij} \tag{2.20}$$

The orientation of grain is updated by transforming two vectors s and n .

$$F_i^e = F(F_i^p)^{-1} \tag{2.21}$$

$$(s_{ij})^* = F_i^e s_{ij}, \quad (n_{ij})^* = n_{ij}(F_i^e)^{-1} \tag{2.22}$$

2.4 Slip velocity model

Gilman[15] suggested the slip velocity model as shown in Eq.(2.23),

$$\dot{\gamma} = 2\,\mathrm{b}\, v_o(\rho_o + \rho\gamma) e^{-\frac{H_o + H_1\gamma}{\tau}} \tag{2.23}$$

where b is Burger's vector, v_o the limit velocity of dislocation, H_o material constant, ρ_o the initial dislocation density, ρ the dislocation increasing rate, and τ resolved shear stress on a slip. H_1 is concerned with a fixed portion of the generated dislocations (actually means hardening). This velocity model is adopted as the base of present model, but some modifications will be given to it.

$H_1\gamma$ is assumed to consist of two ingredients;

$$h_1|\gamma_{ij}^m| + H_i^s \tag{2.24}$$

where h_1 is the material constant, and γ_{ij}^m the maximum slip. H_i^s is given by the following evolution equation.

$$\dot{H}_i^s = c_s(h_s^u - H_i^s)\,\|\dot{\gamma}_i\| \tag{2.25}$$

where c_s is the material constant, h_s^u the saturation value of H_i^s, and $\|\dot{\gamma}_i\|$ is given by the following Eq.(2.26).

$$\| \dot{\gamma}_i \| = \sum_{j=1}^{n_s} | \dot{\gamma}_{ij} | \tag{2.26}$$

The evolution of internal stress due to dislocation substructure is described by

$$\dot{\alpha}_{ij} = c_b (h_b^u - \alpha_{ij}) \dot{\gamma}_{ij} \tag{2.27}$$

where c_b is the material constant, and h_b^u the saturation value of internal stress. Finally introducing power n, the present slip velocity model can be described in detail as follows,

$$\dot{\gamma}_{ij} = sign(\tau_{ij} - \alpha_{ij}) 2\, b\, v_o (\rho_o + \rho | \gamma_{ij}^m |)$$

$$\mathrm{EXP}\left[- \frac{(H_o)^n + (H_s + h_1 | \gamma_{ij}^m |) | \tau_{ij} - \alpha_{ij} |^{n-1}}{| \tau_{ij} - \alpha_{ij} |^n} \right] \tag{2.28}$$

where the shear stress τ_{ij} resolved on slip (ij) is expressed as follows.

$$\tau_{ij} = tr(P_{ij} \sigma) \tag{2.29}$$

3. Simulation of plastic spin

3.1 Material properties and loading condition

The present simulation is performed in an aggregate of body centered crystal which is tried to be a mild steel as far as possible. While Burger's vectors, ρ_o and ρ, are taken from the reference 17), the other material constants are given arbitrarily. If necessary to fit an experimental curve, it can be done by adjusting, first, H_o and n to meet initial yielding, and next the remainder to meet the post-yield curve. The trial material constants are listed in Table 3.1. Initial orientations of grains are shown in Fig.3.1. The markings depict <100> directions of grains. Each point has three grains whose orientations are set by the method of Asaro and Needlmann[18], thus 153 grains are considered in this study.

Table 3.1 Traial material constants

b	2.5E-7 (mm)	v_o	3.2E+6 (mm/s)
ρ_o	375 (mm^{-2})	ρ	1.0E+9 (mm^{-2})
H_o	125 (kg/mm^2)	n	1.35
C_s	30	h_s^u	100 (kg/mm^2)
C_b	12.45	h_b^u	26.5 (kg/mm^2)
h_1	2000 (kg/mm^2)	Poisson Ratio	0.3
Young's Modulus	2.1E+11 (N/m^2)		

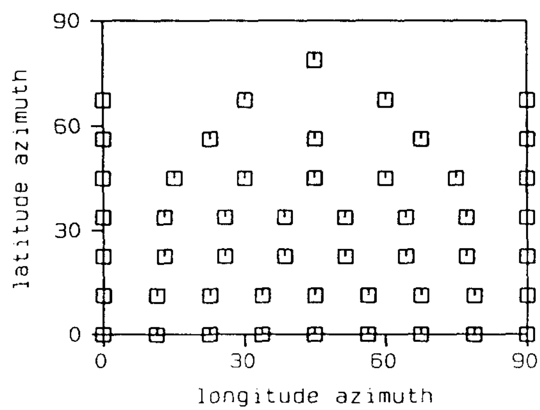

Fig. 3.1 Initial orientaion of grain, <100> direction

The loading is applied by the prescribed increments of deformation gradient which is taken as simple shear,

$$F = \begin{vmatrix} 1 & 0 & 0 \\ \delta t & 1 & 0 \\ 0 & 0 & \delta_{33}^p \end{vmatrix} \tag{3.1.}$$

where δ_{33}^p is the same to the plastic deformation, and t is a time incement. It can be nearly rate-independent plasticity with a small δ. At present, 1.0E-4(/s) and 2.0E2(/s) are used for δ, hereafter called as slow rate and fast rate, respectively.

3.2 Results and discussions

Texturing has been regarded as one of the sources of plastic spin. In what follows, it will be emphasized that texturing is dominant in the plastic spin sources, while the others are secondary. And all discussions below will be done under no polar stress.

Figure 3.2 shows a case of slow rate. The abscissa represents accumulated shear strain. It can be seen that non-dimensional plastic spin (W^p/W) is not asymptotically increasing. This tendency is not similar to the result of Taylor's model in which it is increasing toward 1.0, for instance in Ref. 19). It is manifest that the oscillatory nature of spin ratio depends on the competition between plastic spin and total spin, which means the different tendency comes from the level of plastic spin. Thus two possibilities can be thought; the present simulation gives small plastic spin or Taylor's model gives large plastic spin. The gap can be attributed to the methods of both models for selecting active slip.

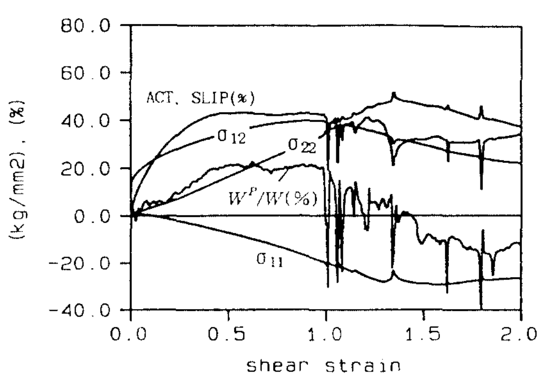

Fig. 3.2 Simulation result for slow rate

Some sharp oscillations in curves of non-dimensional plastic spin and stress may be due to the abrupt changes of active slips. It is well explained by the active slip curve which represents the ratio of slip population currently active to the total slip, where the activation of slip is judged by the criterion $\dot{\gamma} > 10^{-6}(/s)$. Sharp oscillations appear to be well synchronized with those of the active slip curve. In the range of shear strain < 1.0 where there are no sharp fallings in the curve of active slip, such oscillations can not be seen. It is thought that texturing is responsible for those local sharp fallings of active slip population. No such fallings can be found in Fig.3.7 which is obtained under the condition that all grain rotations are forced to be fixed.

On the other hand, Fig. 3.2 shows considerable axial stresses at large strain, especially, σ_{11} is a compression. In some torsion tests, for instances Ref. 20),21), compressive axial stress can be observed while axial movement is prohibited. And it can be also seen the torque and axial stress are fluctuating. The present simulation shows similar behavior to those tests. Referring to Fig.3.7, it can be understood that texturing is an essential factor of those non-coaxial stresses. And the comparison of shear stress curves in Fig.3.2 and Fig.3.7 shows a geometrical softening effect.

Fig.3.3 of the case of fast rate shows similar trends to Fig.3.2, but has less sharp oscillations. Its non-dimensional plastic spin appears higher than that of slow rate. Fig.3.4 shows its comparison between two cases. The fast rate has more delayed point at which the plastic spin changes its direction. This rate dependency will be discussed later.

Hardening effect on the spin ratio is given in Fig.3.5. Dotted curves are reffered to the case of $h_1 = 1000(Kg/mm^2)$ and solid curves, to the

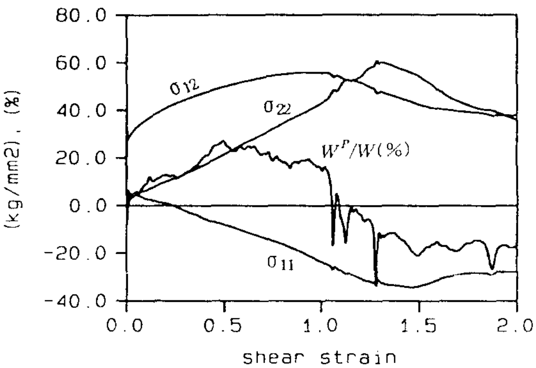

Fig. 3.3 Simulation result for fast rate

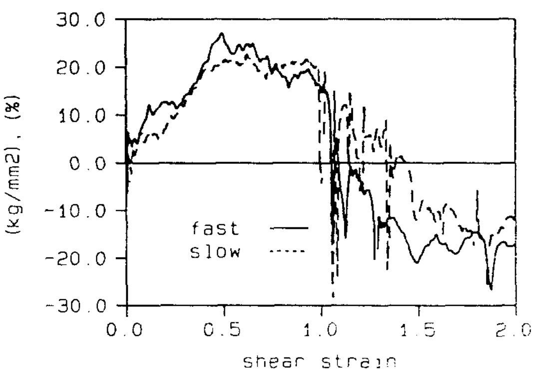

Fig. 3.4 The rate effect

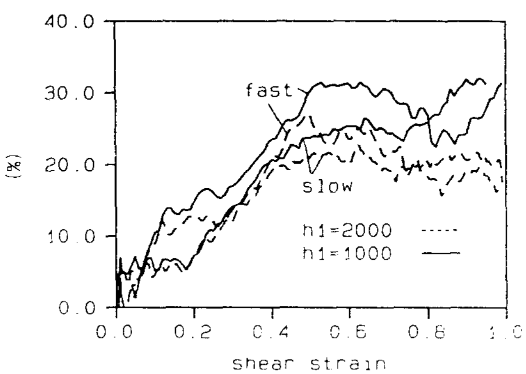

Fig. 3.5 Hardening effect

case of $h_1 = 2000(Kg/mm^2)$. It can be observed the smaller hardening is, the larger non-dimensional plastic spin and rate effect are. Both effects, rate and hardening, can be interpreted in a quarry, overstress; the larger overstress, the larger spin ratio. How larger overstress causes larger non-dimensional plastic spin will be explained later.

The reverse loading effect is also investigated. Its result can be found in Fig.3.6. Just after loading reversed, the spin ratio jumps strikingly and goes down rapidly. While the tension σ_{22} is steeply decreasing to small level, the compression σ_{11} keeps its pace with further rate in a certain range of deformation. It is interesting in the behavior of σ_{11} just after loading is reversed. This behavior as well as the jumping of non-dimensional plastic spin can be explained such that, by back stress, the pattern of active slips is reconstructed to be more amiable to them.

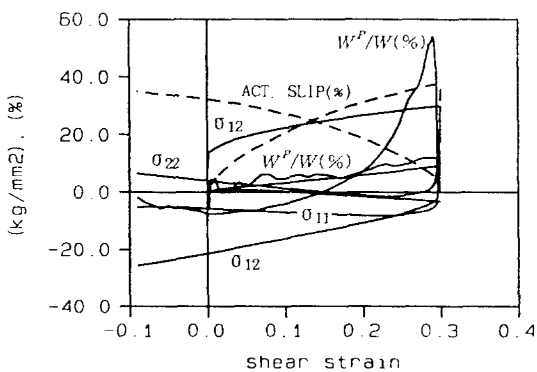

Fig. 3.6 Reverse loading effect

Till now, some phenomena emerged from the present simulation have been described and interpreted. Texturing is crucial, precisely speaking, the textured state of material is. Next it is desiable to enhance it and to gain insight into the plastic spin.

If macroscopic plastic spin(MPS) is regarded as the average of grain spins and grain rotation is evaluated by subtracting grain plastic spin

(GPS) from macroscopic total spin(MTS), it is natural that texturing can be the governing factor for MPS. Here an attention should be given to the fact that neither the conjugate force of texturing nor internal stress(e.g., back stress) is the driving force of plastic spin because it does not urged by such driving forces.

It is useful to classify two spins conceptually; superimposed spin and derived one. While the former is due to rigid body rotation, the latter, to symmetrization. In elasticity, this classification is useless because the distinction can not be measured by material itself and two spins have the same physical meaning. In plasticity, the classification does make sense. It can be deriven with a measurement, anyhow, because the microstructure of material has some information to tell about plastic spin. The plastic spin neither dissipates energy nor has physical meaning. Thus it is not subjected to thermodynamic constraint and there needs no thermodynamic conjugation force. However, texturing dissipates energy so that it has the conjugation force. In fact, the relative rotation of grain to the surrounding, actually giving texturing, is achieved by the deformations such as highly localized deformation in the vicinity of grain boundary and/or crystal twinning[22]

Returning to the origin of plastic spin, it can be considered in two steps; grain level and aggregate one. First, the plastic spin of a grain mainly comes from different levels of induced shear stresses on slips. Boukadia and Sidoroff[23] showed this mechanism analytically. For comprehensive explanation, consider two groups of slip system giving plastic spins with opposite sign each other under the given loading. The resultant plastic spin, namely GPS, is the survivor in the competition between two groups. In this context, the induced shear stress on slip makes a crucial role. The shear stress level of a slip depends on the grain orientation and the combination of stress components. The deformation rate and hardening effect can be outlined as follow. These effects shift the overstresses of slips of both groups to higher levels, and the shifting effect enlarges the unbalance of slip velocity to yield the consequence because of highly accelerated growth in the stress-slip velocity curve.

Second, since MPS is got by averaging whole GPS controlled by grain orientation, the rearranged pattern of its orientation might be a dominant factor as well as the ingredient of stress tensor. From Fig.3.3 and Fig.3.7, it can be seen that these two factors have a greater effect than hardening or rate effect does.

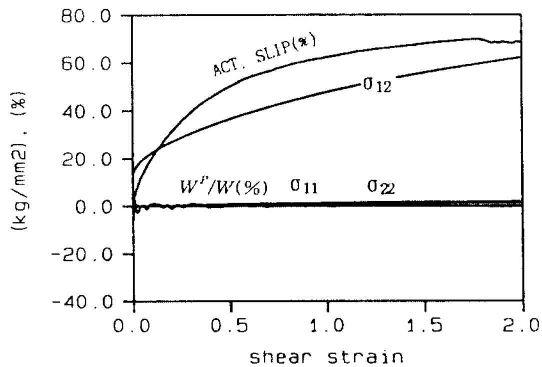

Fig. 3.7 Simulation result for no grain rotation

As what being associated with the effect of stress tensor ingredient, considerable non-coaxial stresses (σ_{11}, σ_{22}) are observed as shown in Fig.3.2 and Fig.3.3. It implies that the non-coaxiality in plasticity is an urgent problem to be tackled. Therefore, all spin models ever suggested might be unfair when the non-coaxiality is considered.

Here are some brief comments to the isotropic function representation(IFR). The back stress is regarded as a parameter representing an arrangement of grain orientation, not a driving force as stressed previously. It can be agreed, to some extent, the back stress is such a parameter. But the current frame of IFR hardly seems to be general enough. It will fail, for example, to follow the plastic spin after the reverse loading as shown in Fig. 3.6 so that IFR wants a modification as well as the non-coaxiality.

Finally, there has issued a debate whether the equation for plastic spin is a constitutive one or a kinematical function. Since Kratochvil[1] recognized the need for another constitutive equation for the plastic spin, several authors have thought of it as a constitutive one. Recently, some authors[12,13] argued that it is a kinematical function. Both seems to be still suspected in the following viewpoints. In spite of the nature of plastic spin discussed so far in this paper and the fact that IFR has a stretch rate, can the equation be regarded as a constitutive equation? Rather a kinematical function? The present simulation and discussion states that the plastic spin can not be given by the complex of kinematic quantities only. In our opinion, it prefers to call such a class of equation as a constitutive kinematic equation or a constitutive constraint.

4. Summary and conclusion

A simple static accommodation model was applied to the simulation of plastic spin of body centered polycrystal in simple shear. The effects, such as texturing, hardening, deformation rate, and reserve loading, were investigated.

The present simulation gives fluctuating non-dimensional plastic spins contrary to Taylor's model. This discordance is expected to lie on the active slip selection method. Texturing itself is not effective on the plastic spin but the rearranged pattern of its orientation is. As a matter of fact, the orientation pattern of grains is a significant factor for the plastic spin. It is also the origin of the considerable non-coaxiality observed in the present simulation. The ingredient of stress tensor and the induced non-coaxiality are the important factors as well as the orientation pattern.

The non-dimensional plastic spin depends on deformation rate and hardening, but these effects are secondhand. The load reversing is followed by the jumping of non-dimensional plastic spin and steep rate of compression. These phenomena can not be described by the existing plastic spin models. Though conventional plastic spin models are thought to be effective to some extent, they are hardly regarded as general ones. Further more they can not be justified until a consideration is given to the induced non-coaxiality.

Finally, without a couple of stresse the plastic spin needs no conjugate force. It also needs not to be subjected to thermodynamic constraint as stated in Ref.24). It should not be confused that the conjugate force of texturing has little effect to the plastic spin in spite of the significant relationship between the plastic spin and texturing. Assumingly the plastic spin may be evaluated independently by a constitutive equation, but it has a relationship with stretch tensor. However, the relations can not be given by the complex of kinematic quantities only. It seems to be preferable to call these classes of equations other titles.

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