



S0749-6419(96)00001-0

AN ANISOTROPIC ELASTIC–PLASTIC CONSTITUTIVE MODEL FOR SINGLE AND POLYCRYSTALLINE METALS. I—THEORETICAL DEVELOPMENTS

A. S. Khan and P. Cheng*

ECS Building 234, University of Maryland, Baltimore County, MD 21228, U.S.A.

(Received in final revised form 15 June 1995)

Abstract—An anisotropic elastic–plastic constitutive model for single and polycrystalline metals is proposed. The anisotropic hardening of single crystals, at first, is discussed with the viewpoint of yield surface and a new formulation of it is proposed. Then, a model for the anisotropic hardening of polycrystals is suggested by increasing the number of slip systems and incorporating the interaction of all slip systems. The interaction of grains through grain boundaries is shown to be similar to, and incorporated into, the interaction of slip systems in grains. The numerical predictions and their comparisons with experiments will follow in Part II of this paper.

I. INTRODUCTION

One of the main features of the stress–strain characteristics of engineering materials is their directional dependency after some plastic deformation, i.e. plasticity-induced anisotropy. To approach this phenomenon, the concept of kinematic hardening has been introduced. Kinematic hardening specifies the center of a yield surface in stress space. As it changes with plastic deformations, the yield surface translates and thus the material has different behaviors in different directions. This approach has been found to be a good approximation of the anisotropic behavior if the plastic deformation is small. The reader is referred to the experimental results by Phillips [1985], Stout [1985], Khan and Wang [1988, 1990] and their applications in constitutive models by Prager [1949], Ziegler [1959], Armstrong and Frederick [1966], Chaboche [1986], Dafalias [1975], Valanis and Lee [1982], among extensive investigations on this topic.

Under finite plastic deformation of about ten percent, experimental data on yield surfaces (see Khan & Wang [1988, 1990]) show that a yield surface changes not only due to translation of its center but also due to distortion of its shape with plastic deformation. In the direction of loading, the yield surface becomes sharp while in the opposite direction of loading, the yield surface tends to become flat. If the loading changes its direction several times, the final yield surface will be composed of several sections with different curvatures. Obviously, this strong anisotropic behavior makes the mathematical representation of such a yield surface very difficult and complicated.

*Currently visiting scholar; permanent address is Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, P.R. China.

For the last few decades, much progress has been made in the study of crystal plasticity (see, e.g. Asaro [1983], Havner [1992]), which gives some valuable insights into the complicated anisotropic behavior of metals. Now it is understood that every point of a yield surface may correspond to the state of one or several slip systems, and the shape of a yield surface may result from the interaction of various slip systems. The large number of slip systems and grain boundaries in polycrystalline metals are responsible for the differences in their yield surfaces compared to those of single crystals. More significantly, studies in crystal plasticity suggest that stress depends not only on strain but also on plastic spin when crystals undergo finite plastic deformation (see, e.g. Havner & Shalaby [1977], Aifantis [1987], Havner [1992] and Dafalias & Aifantis [1992]).

It is desirable to describe the elastic-plastic constitutive relations based on the evolution of the micro-structures. However, this methodology still remains a challenge to researchers with difficulties to be overcome. Various micro-structures and the deformation mechanisms of the engineering materials need to be described, the work hardening of single crystals requires detailed determination. The quantities at the micro-scale level need to be more accurate in relation to those at the macro-scale level, and the theoretical models should be implemented in a practical, numerical manner.

This paper concentrates on a phenomenological model of time-independent plasticity of polycrystalline metals, with emphasis on the description of plasticity-induced anisotropic behavior. It is expected that the developed model will incorporate the important features of crystal plasticity with the conventional formulations of phenomenological theory so that the model will have a sound physical background but will use simple mathematical formulations and numerical analyses. To this end, the experimental observations and theoretical descriptions of the work hardening of single crystals are reviewed in Section II, and then a new representation of the work hardening is discussed and suggested using the concept of a yield surface. Following the consideration of the plastic behavior of single crystals, Section III focuses on the differences between polycrystals and single crystals in their deformation mechanisms, and especially on the role of the large number of slip systems in polycrystals. As a result, the model for single crystals is extended to polycrystals by increasing from a small number of slip systems, say 12 for FCC crystals, to a large number. Section IV analyses the effect of grain boundaries on the behavior of polycrystals and provides an alternative to the self-consistent method proposed by Kroner [1958] and Budiansky and Wu [1962]. The analysis shows that the effect of grain boundaries can be incorporated to the interaction of slip systems formulated in Section III.

II. ANISOTROPIC HARDENING OF SINGLE CRYSTALS

According to the theory of single crystal plasticity developed by Hill [1966], Hill and Rice [1972], Asaro and Rice [1977], Peirce, Asaro and Needleman [1982] and Hill and Havner [1982] (see the review papers given by Asaro [1983] and Havner [1992]), if the plastic behavior of a single crystal is described by

$$\dot{\tau}_c^i = \sum_{j=1}^N h^{ij} \dot{\gamma}^j \quad (1)$$

where $\dot{\tau}_c^i$ and $\dot{\gamma}^i$ are the rates of the critical resolved stress and the slip of the i th slip system, N is the total number of all activated slip systems, and h^{ij} is called work hardening

modulus or hardening for short, and when an external stress acting the single crystal makes the resolved stress and its rate on a slip system, say τ^i and $\dot{\tau}^i$, on the i th slip system satisfy the Schmid criterion:

$$\tau^i = \tau_c^i \quad (2)$$

and the loading condition

$$\dot{\tau}^i = \dot{\tau}_c^i \quad (3)$$

then the slip system will be activated. All the activated slip systems will produce the following plastic velocity gradient:

$$\mathbf{L}^p = \sum_{i=1}^N \mathbf{m}^i \otimes \mathbf{n}^i \dot{\gamma}^i \quad (4)$$

where \mathbf{m}^i and \mathbf{n}^i are the i th slip direction and its plane.

The experimental investigation of the work hardening moduli has attracted many researchers. Among them are Wadsworth [1963], Ramaswami, Kocks and Chalmers [1965], Kocks and Brown [1966], Jackson and Basinski [1967], Basinski (S.J.) and Basinski (Z.S.) [1979], Franciosi, Berveiller and Zaoui [1980] and Franciosi [1983]. Some of the recent reviews of this topic have been given by Kocks [1985] and Bassani [1990]. From these experimental observations, some conclusions about the work hardening moduli seem to be:

- (i) The hardening depends on dislocation structures of materials; FCC crystals show obvious three stage behavior in their resolved stress-strain curves while HPC crystals exhibit low but constantly increasing work hardening (see Honeycombe [1984]);
- (ii) The hardening depends on loading history; plastic deformation changes the dislocation structures. At the initial stage of a plastic deformation, one or several symmetrical slip systems are activated. But after some plastic deformation, cross slips occur and groups of slip systems are activated. If the loading direction is changed, some previously activated slip systems may stop while new slip systems are activated. Every change of the state of slip systems contributes to the interaction of slip systems and causes work hardening moduli to change their values;
- (iii) Self hardening h^{ii} (no sum over i) is somewhat smaller than latent hardening h^{ij} ($i \neq j$); The ratio of latent to self hardening ranges from 1.0 to 1.4;
- (iv) The hardening is anisotropic. The anisotropy comes from two aspects. One is due to the inherent anisotropy of micro-structures. The other aspect is due to the different hardenings on different slip systems after some plastic deformation.

The theoretical study of the hardening started with Taylor's assumption that any activated slip system resulted in the same hardenings on all slip systems. This isotropic model is represented by (see Taylor [1938])

$$h^{ij} = h_i \quad (5)$$

where h_i is a function of stress or plastic deformation. Thus, the self hardening h^{ii} is equal to the latent hardening h^{ij} in this model. Later, Koiter [1963] made another

assumption that every activated slip system caused only self hardening but had no effect on other slip systems. This independent hardening model means

$$h^{ij} = h_k \delta^{ij} \quad (6)$$

where h_k is a function of stress or plastic deformation, and δ^{ij} is the Kronecker delta. The two assumptions are, of course, not accurate enough to describe the above experimental phenomena. Hutchinson [1970] and Asaro [1983] proposed the following mixed model

$$h^{ij} = qh_h + (1 - q)h_h \delta^{ij} \quad (7)$$

where q ranges from 1.0 to 1.4 and represents the ratio of latent hardening to self hardening. But this mixed model still can not describe the observed anisotropic behavior. Budiansky and Wu [1962] and Weng [1979] extended Taylor's isotropic model to anisotropic models by adding kinematic hardening. Budiansky and Wu [1962] proposed that

$$h^{ij} = h_{b0} + h_{b1} \mathbf{P}^i : \mathbf{P}^j \quad (8)$$

where h_{b0} and h_{b1} are two functions of stress or plastic deformation, and \mathbf{P}^i is the symmetric part of $\mathbf{m}^i \otimes \mathbf{n}^i$. Weng [1979] suggested:

$$h^{ij} = qh_w + (1 - q)h_w \cos \theta^{ij} \cos \phi^{ij} \quad (9)$$

where θ^{ij} is the angle between the slip directions of the i th and j th systems, ϕ^{ij} is the angle between their slip planes and h_w is a function of stress or plastic deformations. Budianski and Wu's model is very similar to Prager's rule for the kinematic hardening in the phenomenological theory of plasticity. By noting

$$\tau^i = \mathbf{P}^i : \boldsymbol{\sigma} \quad (10)$$

where $\boldsymbol{\sigma}$ is Cauchy stress, eqn (8) and the rate form of eqn (2) can be rewritten for infinitesimal deformation as

$$\mathbf{P}^i : (\dot{\boldsymbol{\sigma}} - \dot{\mathbf{x}}_w) = h_{b0} \sum_j \dot{\gamma}^j \quad (11)$$

where

$$\dot{\mathbf{x}}_w = h_{b1} \mathbf{D}^p \quad (12)$$

where \mathbf{D}^p is the plastic strain rate defined by the symmetrical part of \mathbf{L}^p . Weng's model produces an obvious physical interpretation that the hardenings caused by cross slips depend on the angles of slip directions and planes. More recently, Bassani and Wu [1989] (see Bassani [1990]) proposed that

$$h^{ii} = h_b, \quad (\text{no sum over } i) \quad (13)$$

$$h^{ij} = mh_b, \quad (i \neq j) \quad (14)$$

where h_b is a function of the up-dated state of crystals and m is a constant. Moreover, Havner and Shalaby [1977] (see Havner [1992]) took the rotation caused by slips into consideration and proposed that

$$h^{ij} = h - 2tr(\mathbf{P}^i \cdot \boldsymbol{\sigma} \cdot \mathbf{Q}^j) \quad (15)$$

where \mathbf{Q}^j is the anti-symmetrical part of $\mathbf{m}^j \otimes \mathbf{n}^j$. And similarly, Peirce, Asaro and Needleman [1982] proposed that

$$h^{ij} = h - tr(\mathbf{P}^i \cdot \boldsymbol{\sigma} \cdot \mathbf{Q}^j) - tr(\mathbf{Q}^i \cdot \boldsymbol{\sigma} \cdot \mathbf{P}^j) \quad (16)$$

The two rotation-dependent models reduce to Taylor's isotropic model if the rotation is neglected.

It is helpful to understand these models in terms of a yield surface. Figure 1 depicts the movements and changes of a yield surface caused by the elements of these models. In Fig. 1, (a) shows the Taylor isotropic hardening, (b) shows the kinematic hardening in the models of Budiansky and Wu [1962] and Weng [1979], and (c) shows the Kroner independent hardening. In addition, by considering that the yield surface may not be the combination of the three kinds of hardenings, Fig. 1 (d) illustrates a more general case that the yield surface changes in its shape, becoming sharper in the loading direction and flatter in the opposite direction.

According to these considerations, a new model of the hardening is outlined as follows:

(i) Because the anisotropic behavior may be the main difficulty to model the hardening of single crystals, it is natural to consider the hardening of slip systems individually. For every slip system, after some plastic deformation the critical resolved shear stress in the forward direction is generally different from that in the backward direction. That is, every slip system may have some Bauschinger effect after some slip of the

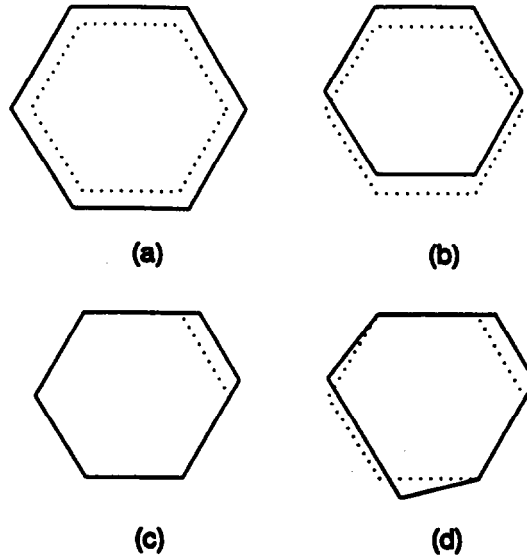


Fig. 1. Evolution of Yield Surface (a) Isotropic Hardening, (b) Kinematic Hardening (c) Independent Hardening and (d) General Hardening.

slip system, or another slip system. Therefore, we introduce the concept of kinematic and isotropic hardenings to every slip system such as

$$|\tau^i - x^i| \leq r^i + \tau_0 \quad (17)$$

where x^i and r^i are the kinematic and isotropic hardenings of the i th slip system, respectively, and τ_0 is the initial critical shear stress.

The use of the two different hardenings, rather than forward and backward yield stresses, simplifies the representation of the interacting hardenings among slip systems. In terms of yield stress, it is necessary to represent the interaction, say of the i th slip system to the j th slip system, as a function of their relative location $\mathbf{P}^i : \mathbf{P}^j$. Due to a possible wide variety of loading histories, this function may be very complicated. But in terms of the kinematic and isotropic hardenings, it is understood by their definitions that the kinematic hardening should be an odd function of relative location $\mathbf{P}^i : \mathbf{P}^j$, and the isotropic hardening should be an even function of $\mathbf{P}^i : \mathbf{P}^j$.

(ii) As for the relative location $\mathbf{P}^i : \mathbf{P}^j$ between the i th and the j th slip systems, there are two possibilities. One is that the two slip systems are in one slip plane, i.e. coplanar slip systems. The other possibility is that the two slip systems are not coplanar, i.e. forest slip systems. The experiments on the hardening of single crystals show that the two kinds of slip systems have different interactions. Bassani [1990] pointed out that forest slip systems have stronger hardening than coplanar slip systems. Therefore, the evolution of kinematic and isotropic hardening of every slip system is expected to be

$$\dot{x}^i = \sum_j \dot{\gamma}^j F_p(\mathbf{P}^i : \mathbf{P}^j) + \sum_j \dot{\gamma}^j F_f(\mathbf{P}^i : \mathbf{P}^j) \quad (18)$$

and

$$\dot{r}^i = \sum_j \dot{\gamma}^j G_p(\mathbf{P}^i : \mathbf{P}^j) + \sum_j \dot{\gamma}^j G_f(\mathbf{P}^i : \mathbf{P}^j) \quad (19)$$

where subscripts p and f represent coplanar and forest slip systems and F and G are odd and even functions of their arguments.

(iii) Functions F_p , F_f , G_p and G_f are generally very complicated. They depend not only on the relative locations but also on deformation history. In the above expression of these functions, deformation history is not explicitly listed as an argument, since the present priority is on formulating the interaction of slip systems. In general, the functions of the relative locations could be expected to be smooth enough and be approximated by polynomials. Thus, it is assumed that

$$F_p = a_1^p \xi + a_3^p \xi^3 + a_5^p \xi^5 + \dots \quad (20)$$

$$F_f = a_1^f \xi + a_3^f \xi^3 + a_5^f \xi^5 + \dots \quad (21)$$

$$G_p = a_0^p + a_2^p \xi^2 + a_4^p \xi^4 + \dots \quad (22)$$

and

$$G_f = a_0^f + a_2^f \xi^2 + a_4^f \xi^4 + \dots \quad (23)$$

where ξ is $\mathbf{P}^i : \mathbf{P}^j$ and all the coefficients depend on deformation history. For FCC crystals, the initial values of ξ are -0.25 , -0.0833 , 0.1666 , 0.3333 and 0.5 . Of course, to obtain a practical model, the terms of these functions should be limited; the fewer the terms, the simpler the model. Moreover, if every term has some physical interpretation, it may be helpful to determine the coefficients from material experimental data. In order to find an optimum number of terms, let us discuss the specific cases of the functions.

(i) If $F_p = 0$, $F_f = 0$, $G_p = a_0^p$ and $G_f = a_0^f$, where a_0^p and a_0^f depend on stress or plastic deformation history, or in other words, if the kinematic hardening is assumed to be zero and the isotropic hardening is taken to be first order, then eqn (19) reduces to

$$\dot{r}^i = (a_0^p + a_0^f) \sum_j \dot{\gamma}^j \quad (24)$$

This is just the Taylor isotropic model.

(ii) If $F_p = a_1^p \xi = a_1^p \mathbf{P}^i : \mathbf{P}^j$, $F_f = a_1^f \xi = a_1^f \mathbf{P}^i : \mathbf{P}^j$, $G_p = 0$ and $G_f = 0$, where a_1^p and a_1^f depend on stress or plastic deformation history, or the kinematic hardening is assumed to be first order but the isotropic hardening is assumed to be zero, then the yield condition eqn (17) can be rewritten as

$$|\mathbf{P}^i : (\boldsymbol{\sigma} - \mathbf{x})| \leq \tau_0 \quad (25)$$

where

$$\dot{\mathbf{x}} = (a_1^p + a_1^f) \mathbf{D}^p \quad (26)$$

This is a pure kinematic hardening model, similar to Prager–Ziegler’s linear kinematic hardening model, the same as Budiansky and Wu’s linear kinematic hardening model when a_1^p and a_1^f are constants, and is almost the same as Weng’s kinematic hardening model in the representation of the relative locations of slip systems.

(iii) The combination of above two cases yields a mixed model with isotropic and kinematic hardenings.

From this discussion, two things seem clear. One, the first term of these functions is the first order approximation to the hardening of single crystals, since it is known from crystal plasticity and the phenomenological theory of plasticity that kinematic and isotropic hardenings (which in these cases are state variables rather than slip-related variables) are a good approximation to plasticity-induced anisotropic behavior. They describe the change in size and position of a yield surface. Second, the terms with higher order must be included in the polynomials if the anisotropic behavior, e.g. the change of a yield surface in shape, is to be described more accurately.

(iv) Based on the above analyses, it seems appropriate to assume that the polynomials have two terms, i.e.

$$F_p \sim a_1^p \xi + a_3^p \xi^3 \quad (27)$$

$$F_f \sim a_1^f \xi + a_3^f \xi^3 \quad (28)$$

$$G_p \sim a_0^p + a_2^p \xi^2 \quad (29)$$

and

$$G_f \sim a_0^f + a_2^f \xi^2 \quad (30)$$

with the first terms describing the change of a yield surface in its size and center, and the second terms representing the change of a yield surface in its shape.

(v) Moreover, it seems necessary to add the Koiter independent (self) hardening to the above consideration. It is known that Koiter's and Hutchinson's models provide for a unique relation between slips and resolved shear stresses. The uniqueness is important at least in the numerical implementation of a model. Further, the addition of this independent hardening provides a more accurate description of the kinematic hardening. Generally speaking, the kinematic hardening of a slip system is an odd function of its relative positions to all other activated slip systems. In the above equations, for simplicity, only the first two terms of the polynomials are retained, but any small error due to neglect of high order terms is more than compensated by the inclusion of the independent hardening.

By adding the independent hardening to eqns (27) and (28), the isotropic and kinematic hardenings will take the forms:

$$\dot{x}^i \sim a \dot{\gamma}^i + \sum_j \dot{\gamma}^j \left(a_1 \mathbf{P}^i : \mathbf{P}^j + a_3 (\mathbf{P}^i : \mathbf{P}^j)^3 \right) \quad (31)$$

and

$$\dot{r}^i \sim \sum_j \dot{\gamma}^j \left(a_0 + a_2 (\mathbf{P}^i : \mathbf{P}^j)^2 \right) \quad (32)$$

in which j is summed over all activated slip systems, a_k ($k = 0,1,2,3$) represents a_k^f for coplanar slip systems and a_k^f for forest slip systems.

(vi) In the considerations above, the emphasis is put on the description of the interaction of slip systems. Quantities a and a_k ($k = 0,1,2,3$) are not specified. If these quantities are assumed to be material parameters, i.e. independent of stress and deformation, the kinematic and isotropic hardenings will be linear functions of activated slips. Experiments on single crystals (see, e.g. Wadsworth [1963] and Honeycombe [1984]) show that single crystals normally have three stages in their resolved stress-strain curves. During the first stage, the magnitude of the hardening is small and almost linear. During the second and third stages, the hardening is significant and nonlinear. Especially, when the deformation is finite, the resolved shear stress reaches a saturated value. If the loading is reversed, the yield stress and hardening will be much different from those during the initial loading. It is obvious that for the stage one stress-strain relation, quantities a_k may be assumed to be constants. It means that for $\tau^i < \tau_1$, where τ_1 is the resolved shear stress at the end of the stage one loading, the hardenings are assumed to be

$$\dot{x}^i = a \dot{\gamma}^i + \sum_j \dot{\gamma}^j \left(a_1 \mathbf{P}^i : \mathbf{P}^j + a_3 (\mathbf{P}^i : \mathbf{P}^j)^3 \right) \quad (33)$$

and

$$\dot{r}^i = \sum_j \dot{\gamma}^j \left(a_0 + a_2 (\mathbf{P}^i : \mathbf{P}^j)^2 \right) \quad (34)$$

where a and a_k ($k = 0,1,2,3$) are constants. In terms of the work hardening moduli, the combination of eqns (33), (34) and the rate of eqn (17) yields

$$\tau^i < \tau_c^i = \sum_j h^{ij} \dot{\gamma}^j \quad (35)$$

where

$$h^{ij} = a \delta_{ij} + a_1 \mathbf{P}^i : \mathbf{P}^j + a_3 (\mathbf{P}^i : \mathbf{P}^j)^3 + \text{sign}(\tau^i - x^i) (a_0 + a_2 (\mathbf{P}^i : \mathbf{P}^j)^2) \quad (36)$$

with $\text{sign}(z) = 1$ if $z > 0$ and $\text{sign}(z) = -1$ if $z < 0$.

For the last two stages, quantities a_k may be taken to be functions of stress or strain to describe the observed nonlinearity. These functions can not represent the change of the hardening when loading is reversed. An alternative approach is to use the method proposed by Armstrong and Frederick [1966]. The quantities are assumed to be constants, but feedback terms are added to the above formulation describing the hardenings. That is, for the last two stages and loading reversals, the hardenings are assumed to be

$$\dot{x}^i = \sum_j b_x \dot{\gamma}^j (X_0 \delta^{ij} + X_1 \mathbf{P}^i : \mathbf{P}^j + X_3 (\mathbf{P}^i : \mathbf{P}^j)^3 - x^i) \quad (37)$$

and

$$\dot{r}^i = \sum_j b_r \dot{\gamma}^j (R_0 + R_2 (\mathbf{P}^i : \mathbf{P}^j)^2 - r^i) \quad (38)$$

where constants a and a_k have been replaced by constants $X_0, X_1, X_3, R_0, R_2, b_x$ and b_r . Constants X_0, X_1, X_3, R_0 and R_2 are the saturated values of the corresponding hardenings, and b_x and b_r are the shape-controlled parameters. In terms of the work hardening moduli, this evolution of the isotropic and kinematic hardenings will give the following work hardening moduli:

$$\begin{aligned} h^{ij} = & b_x (X_0 \delta_{ij} + X_1 \mathbf{P}^i : \mathbf{P}^j + X_3 (\mathbf{P}^i : \mathbf{P}^j)^3 - x^i) \\ & + \text{sign}(\tau^i - x^i) b_r (R_0 + R_2 (\mathbf{P}^i : \mathbf{P}^j)^2 - r^i) \end{aligned} \quad (39)$$

If coplanar slip systems are distinguished from forest slip systems, all the constants in the above equations may have different values for different types of slip systems.

III. A PHENOMENOLOGICAL MODEL FOR POLYCRYSTALS

Polycrystals are aggregates of single crystal grains. Every grain is located in an aggregate with its own shape, size and orientation so that polycrystals are inhomogeneous in their micro-structures. The aggregation and the inhomogeneity make the stress-strain relations of polycrystals different from those of single crystals in many respects.

Due to the aggregation, a polycrystal behaves like the average of single crystals so that an average method, e.g. the volume average method, must be used to describe the

behavior of a polycrystal, as based on the behavior of single crystals. The behavior of a polycrystal will depend on the inhomogeneous shapes, sizes and orientations of the single crystal grains. And more significantly, these differences result in inhomogeneous deformations and stresses in single crystal grains. Thus, the behavior of a polycrystal is the result of the interaction of single crystal grains, usually called the grain boundary effect although grain boundary effect also refers to the different micro-structures of single crystal grains near their boundaries.

In order to describe the behavior of polycrystals on the basis of the responses of single crystals, many researchers have advanced simplified formulations. To avoid the difficulty of relating the behavior of a polycrystal to the shapes and sizes of single crystal grains, the orientation average method (see, e.g. Hutchinson [1970]) is used for an alternative to the commonly used volume average method. To account for the inhomogeneous deformations of single crystal grains, the self consistent method proposed by Kroner [1958], Budiansky and Wu [1962] is adopted. In the self consistent method, the interaction of single crystal grains is simplified as an Eshelby inclusion problem.

In our opinion, while it is worthwhile to consider the interaction of single crystal grains in detail and especially to consider the simpler formulation of the behavior of polycrystals for the cases of complex loading history, it is equally valuable to investigate a practical constitutive model of polycrystals by incorporating the deformation mechanisms of single crystals into the advances in the phenomenological theory of plasticity.

It is known that the plastic deformations of polycrystals are caused by slips of single crystals within them. Compared with a single crystal, a polycrystal contains a much larger number of slip systems, which are randomly distributed in the polycrystal. If the orientation average method, rather than volume average method, is used, the orientations of slip systems are included in the behavior of polycrystals; the shape and size effects are ignored. Moreover, due to the grain boundary effect, all slip systems interact with one another. Describing the behavior of polycrystals means formulating the interaction of all slip systems.

From the phenomenological point of view, the plastic behavior of polycrystals is anisotropic after some plastic deformation. The anisotropy depends on the magnitude of deformation and deformation history. The larger the deformation and the more complex the loading history, the stronger the anisotropy will be. In terms of a yield surface, the yield locus is in general very complicated in shape. To describe the anisotropic behavior, isotropic and kinematic hardenings were introduced to represent the average change of a yield surface in size and center. It is known that these hardenings are a first order approximation to a yield surface in a sense of the average size and general shape of the yield surface. To more accurately describe the anisotropic behavior, a commonly used method is to add internal variables, see, e.g. Chaboche [1986]. It is obvious that as more internal variables are used, the description will become more accurate. This method will not be practical in dealing with the strong anisotropic behavior of polycrystals, since there are many different behaviors in different directions and their representation requires many internal variables. To get a general description of the anisotropy, it seems appropriate to introduce direction-dependent variables, rather than state-dependent variables such as kinematic hardening. There should be as many direction-dependent variables as needed to represent the strong anisotropy under finite deformation and complex deformation history.

By combining the considerations above on the deformation mechanisms and the phenomenological description of the plastic behavior of polycrystals, and by noting that slip systems are direction-dependent variables, it is suggested that the plastic deformation of polycrystals can be modeled as a large number of randomly distributed slip systems.

To represent such a large number of randomly distributed slip systems, one way is to use the three Euler angles β , θ and ϕ to express a slip plane and a slip direction such that

$$\mathbf{n} = (\sin\theta \cos\beta, \sin\theta \sin\beta, \cos\theta) \quad (40)$$

and

$$\mathbf{m} = (-\cos\theta \cos\beta \sin\phi - \sin\beta \cos\phi, -\cos\theta \sin\beta \sin\phi + \cos\beta \cos\phi, \sin\theta \sin\phi) \quad (41)$$

where $0 \leq \theta \leq \frac{\pi}{2}$, $0 \leq \beta \leq 2\pi$ and $0, \leq \phi \leq 2\pi$. When β , θ and ϕ are taken to be a number of discrete values (see, e.g. Liang & Cheng [1993]), say L , M and N values, respectively, there are $L \times M$ slip planes, and on each slip plane there are N slip directions. Further, let

$$\mathbf{P} = \frac{1}{2}(\mathbf{m} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{m}) \quad (42)$$

denote a slip system, then the number of slip systems will be $L \times M \times N$.

Analogous to the case of single crystals, the central issue in describing the plastic behavior of polycrystals is to formulate the interaction of slip systems. To this end, the same ideas and method will be used here as for single crystals. Let r^i and x^i denote the isotropic and kinematic hardenings of the i th slip system which satisfy the following condition:

$$|\tau^i - x^i| \leq r^i + \tau_0 \quad (43)$$

where τ_0 is the initial critical shear stress and

$$\tau^i = \mathbf{P}^i : \boldsymbol{\sigma} \quad (44)$$

is the resolved stress on the i th slip system.

As in the analyses of the isotropic and kinematic hardenings for single crystals, the evolution of the hardenings x^i and r^i with plastic deformation can be assumed to be proportional to the slip rates, and even and odd functions of relative location $\mathbf{P}^i : \mathbf{P}^j$ to the j th slip system, respectively. Especially when these functions are assumed to be polynomials, their first terms will correspond to the state-related isotropic and kinematic hardenings in the conventional models of phenomenological constitutive relations such as given by Chaboche [1986]. Their second terms will correspond to the shape change of a yield surface. Therefore, the polynomials are assumed to consist of two terms. Further, the coefficients of the two terms may be taken to be constants, if the isotropic and kinematic hardenings are assumed to be linear with respect to the slips. But most experimental data on polycrystals show that the hardenings are normally nonlinear with plastic deformations. In fact, the hardening is nonlinear and different from that in the initial loading direction when the loading direction is reversed. These experimental

results are quite similar to the second and third stage hardenings of single crystals. Thus, following the approach adopted for the second and third stage hardenings of single crystals, the coefficients are assumed to be constants but feedback terms are added to the polynomials. That is, the isotropic and kinematic hardenings are assumed to be

$$\dot{x}^i = \sum_j^N b_x \dot{\gamma}^j \left(X_0 \delta^{ij} + X_1 \mathbf{P}^i : \mathbf{P}^j + X_3 (\mathbf{P}^i : \mathbf{P}^j)^3 - x^i \right) \quad (45)$$

and

$$\dot{r}^i = \sum_j^N b_r \dot{\gamma}^j \left(R_0 + R_2 (\mathbf{P}^i : \mathbf{P}^j)^2 - R^i \right) \quad (46)$$

where b_x , X_1 , X_3 , b_r , R_0 , R_2 and X_0 are material constants. Again, constants X_0 , X_1 , X_3 , R_0 and R_2 are saturated values of corresponding hardenings, and b_x and b_r are the shape-controlled parameters.

IV. CONSIDERATION OF GRAIN BOUNDARY EFFECTS

In the preceding section, the behavior of polycrystals was described based solely on slip systems. The grain boundary effect is another important aspect in the plastic behavior of polycrystals. As explained in the beginning of the last section, the orientation average method neglects the effect which the size and shape of single crystals has on the behavior of their aggregate. Also, only direction-dependent quantities should be used to represent the anisotropic behavior of polycrystals. Therefore, the grain boundary effect enters the polycrystal model indirectly through the interaction of slip systems. For example, in a polycrystal containing 100 FCC single crystal grains, the maximum number of interacting slip systems is 1200; if the grain boundary effect is neglected, the number of interacting slip systems would be only 12. In order to illustrate this concept quantitatively, we proceed with an alternative, but more traditional analysis.

Let the subscripts g and l distinguish global quantities from local ones. For instance, σ_g and σ_l are the global and local stresses, respectively. According to the orientation average

$$\langle \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} d\beta \int_0^\pi \sin\theta d\theta \int_0^{2\pi} (\) d\phi \quad (47)$$

for polycrystals, global stress and strain should satisfy the following relations.

$$\sigma_g = \langle \sigma_l \rangle, \quad \dot{\sigma}_g = \langle \dot{\sigma}_l \rangle \quad (48)$$

and

$$\mathbf{D}_g^p = \langle \mathbf{D}_l^p \rangle \quad (49)$$

Because of the grain boundary effect, deformation and stress will not be uniform in a polycrystal. Every grain has its own stresses and deformations which are different from

those of the aggregate. Let \mathbf{x} denote the difference of a local stress at a grain from the global stress such that

$$\mathbf{x} = \boldsymbol{\sigma}_g - \boldsymbol{\sigma}_l \quad (50)$$

then \mathbf{x} specifies the residual or back stress at the grain caused by neighboring grains around it. From eqn (48),

$$\langle \mathbf{x} \rangle = 0 \quad (51)$$

that is, the back stresses in grains have no effect on global stress.

\mathbf{x} is expected to be related to the difference of plastic deformation, $\mathbf{D}_l^p - \mathbf{D}_g^p$. If no difference in plastic deformation appears in the polycrystal, the deformation will be uniform and no back stress exists. As the first order approximation for infinitesimal deformation without loss of its generality, the rate of the back stress at a grain may be assumed to be proportional in its magnitude and identical in its direction to the difference of the plastic strain rate of the grain from the global one, such as

$$\dot{\mathbf{x}} = A(\mathbf{D}_g^p - \mathbf{D}_l^p) \quad (52)$$

where A is a function of stress or plastic deformation. It is obvious that eqn (52) satisfies the condition of eqn (51), if the initial value of \mathbf{x} is zero.

With this consideration of grain boundary effect, the yield criterion eqn (17) for every grain becomes:

$$|\mathbf{P}^i : \boldsymbol{\sigma}_g - \mathbf{x}^i| = r_l^i \quad (53)$$

$$\mathbf{x}^i = \mathbf{P}^i : \mathbf{x} + x_l^i \quad (54)$$

By using eqns (37), (38) and (52), the evolution equations of x^i and r_l^i are found to be

$$\dot{x}^i = A\mathbf{P}^i : (\mathbf{D}_g^p - \mathbf{D}_l^p) + \sum_{j_l}^N b_x \dot{\gamma}^{j_l} \left(X_0 \delta^{i j_l} + X_1 \mathbf{P}^i : \mathbf{P}^{j_l} + X_3 (\mathbf{P}^i : \mathbf{P}^{j_l})^3 - x^i \right) \quad (55)$$

and

$$\dot{r}_l^i = \sum_{j_l}^N b_r \dot{\gamma}^{j_l} \left(R_0 + R_2 (\mathbf{P}^i : \mathbf{P}^{j_l})^2 - R^i \right) \quad (56)$$

where j_l represents the local sum over the activated slip systems in the grain which contains the i th slip system. Furthermore, if \mathbf{D}_g^p is calculated in such a way that

$$\mathbf{D}_g^p = \langle \mathbf{D}_l^p \rangle = \sum_{\beta} \sum_{\theta} \sum_{\phi} w \sum_i \mathbf{P}^i \dot{\gamma}^i = \sum_j w \mathbf{P}^j \dot{\gamma}^j \quad (57)$$

where $w = \frac{\Delta\beta\Delta\theta\Delta\phi\sin\theta}{8\pi^2}$ and j is the global sum over all activated slip systems, then eqns (55) and (56) can be rewritten as

$$\begin{aligned} \dot{x}^i = & A \sum_{j_i} (w-1) \mathbf{P}^i : \mathbf{P}^j \dot{\gamma}^j + A \sum_{j_{g-1}} w \mathbf{P}^i : \mathbf{P}^j \dot{\gamma}^j \\ & + \sum_{j_i}^N b_x \dot{\gamma}^j \left(X_0 \delta^{ij} + X_1 \mathbf{P}^i : \mathbf{P}^j + X_3 (\mathbf{P}^i : \mathbf{P}^j)^3 - x^i \right) \end{aligned} \quad (58)$$

and

$$\dot{r}_i^i = \sum_j^N b_r \dot{\gamma}^j \left(R_0 + R_2 (\mathbf{P}^i : \mathbf{P}^j)^2 - R^i \right) \quad (59)$$

where j_{g-1} represents the sum over all activated slip systems except j_i .

Equations (58) and (59) show that the grain boundary effect indeed enters the kinematic hardening model through the interaction of slip systems in all grains but does not change the isotropic hardening. The expressions are very similar in format to eqns (45) and (46), if the first and second terms of eqn (58) are combined with the last term, even though the coefficients in eqn (58) are different from those in eqn (45). Further, formulations in the previous section are easier to use compared to eqns (58) and (59). Therefore, eqns (45) and (46) should be preferred in engineering applications.

V. CONCLUDING REMARKS

1. In order to describe the plasticity-induced anisotropic behavior of polycrystals, the plastic deformation of polycrystals can be attributed to the activation of a large number of randomly distributed directors. The directors were assumed to be identical with slip systems in this paper, and thus the theories of plasticity for single crystals were applied to polycrystals except that the model for polycrystals includes a large number of slip systems.

2. To represent the interaction of slip systems, or directors in a general sense, the evolution of the isotropic and kinematic hardenings, i.e. the forward and backward critical shear stresses, of a slip system were assumed to be proportional to the rates of slips, and the even and odd polynomial functions of the first two degrees, respectively, of the relative locations of the slip system to all activated slip systems. It was shown that the first terms of the two polynomials corresponded, respectively, to the Taylor [1938] isotropic hardening, and the Budiansky and Wu [1962] or the Weng [1979] kinematic hardening. The second terms of the two polynomials were the first order approach to the shape change of a yield surface due to the isotropic and kinematic hardenings of each slip system.

3. To account for the dependence of the plastic behavior of slip systems on deformation history, a feedback term used by Armstrong and Frederick [1966] in their model of nonlinear kinematic hardening was added to each of the polynomial expressions for the isotropic and kinematic hardenings of a slip system.

4. To show the credibility of the extension from single crystals to polycrystals by simply increasing the number of slip systems, an alternative analysis to the self-consistent method proposed by Kroner [1958] and Budiansky and Wu [1962] was proposed to consider the effect of grain boundaries on the behavior of polycrystals. The analysis concluded that the effect of grain boundaries could be incorporated to the interaction of slip systems.

Acknowledgment—The financial support of the National Science Foundation, through grant No. MSS-9296057, Mechanics and Materials Program, is sincerely appreciated.

REFERENCES

- 1938 Taylor, G.I., "Plastic Strain in Metals", *J. Inst. Metals*, **62**, 307.
- 1949 Prager, W., "Recent Developments in the Mathematic Theory of Plasticity", *J. Appl. Phys.*, **20**, 235.
- 1957 Seeger, A., Diehl, J., Mader, S. and Rebstock, H., "Work Hardening and Work Softening of Face-Centred Cubic Metal Crystals", *Phil. Magazine*, **2**, 323.
- 1958 Kroner, E., "Berechnung der Elastischen Konstanten des Vielkristalls aus den Konstanten des Einkristalls", *Z. Phys.*, **151**, 504.
- 1959 Ziegler, H., "A Modification of Prager's Hardening rule", *Quart. Appl. Math.*, **17**, 55.
- 1962 Budiansky, B. and Wu, T.T., "Theoretical Prediction of Plastic Strain of Polycrystals", *Proc. 4th U.S. Nat. Congr. Appl. Mech.*, 1175.
- 1962 Philips, W.L., Jr., "Aluminum and Copper Tested in Direct Shear", *Trans. Metall. Soc. AIME*, **224**, 845.
- 1963 Wadsworth, N.J., "Work Hardening of Copper Crystals under Cyclic Straining", *Acta Metall.*, **11**, 663.
- 1964 Kocks, U.F., "Latent Hardening and Secondary Slip in Aluminum and Silver", *Trans. Metall. Soc. AIME*, **230**, 1160.
- 1964 Ramaswami, B., Kocks, U.F. and Chalmers, B., "Latent Hardening in Silver and an Ag-Au Alloy", *Trans. of the Metall. Society of AIME*, **233**, 927.
- 1965 Hill, R., "Continuum Micro-Mechanics of Elastoplastic Polycrystals", *J. Mech. Phys. Solids*, **13**, 89.
- 1966 Armstrong, P.J. and Frederick, C.O., "A Mathematical Representation of the Multi-axial Bauschinger Effect", G.E.G.B. Report RD/B/N 731.
- 1966 Kocks, U.F. and Brown, T.J., "Latent Hardening in Aluminum", *Acta Metall.*, **14**, 87.
- 1966 Nakada, Y. and Keh, A.S., "Latent Hardening in Iron Single Crystals", *Acta Metall.*, **14**, 961.
- 1967 Hirsch, P.B. and Mitchell, T.E., "Stage II Work Hardening in Crystals", *Canadian J. Physics*, **45**, 663.
- 1967 Jackson, P.J. and Basinski, Z.S., "Latent Hardening and the Flow Stress in Copper Single Crystals", *Canadian J. of Physics*, **45**, 707.
- 1970 Hutchinson, J.W., "Elastic-Plastic Behavior of Polycrystalline Metals and Composites", *Proc. Roy. Soc. Lond.* **A319**, 247.
- 1971 Takeuchi, T and Mano, J., "Latent Hardening in Iron Single Crystals with [110] Extension Axis", *Acta Metall.*, **20**, 809.
- 1971 Valanis, K.C., "A Theory of Viscoplasticity Without a Yield Surface, Part I: General Theory", *Arch. Mech.*, **23**, 517.
- 1976 Dafalias, Y.F. and Popov, E.P., "Plastic Internal variables Formulism of Cyclic Plasticity", *ASME J. Appl. Mech.*, **43**, 645.
- 1977 Havner, K.S. and Shalaby, A.H., "A Simple Mathematical Theory of Finite Distortional Latent hardening in Single Crystals", *Proc. Roy. Soc. Lond.*, **A358**, 47.
- 1979 Basinski, S.J. and Basinski, Z.S., "Work Hardening of Single Crystals", *Dislocation in Solids*, Ed. by Nabarro, F.R.N., Amsterdam, 263.
- 1979 Weng, G.J., "Kinematic Hardening Rule in Single Crystals", *Int. J. Solids and Structures*, **15**, 861.
- 1980 Franciosi, P., Berveiller, M. and Zaoui, A., "Latent Hardening in Copper and Aluminum Single Crystals", *Acta Metall.*, **28**, 273.
- 1982 Valanis, K.C., and Lee, C.F., "Some Recent Developments of the Endochronic Theory with Application", *Nuclear Engineering and Design*, **69**, 327.
- 1983 Asaro, R.J., "Micro-mechanics of Crystals and Polycrystals", *Advances in Mechanics*, **23**, 1.
- 1983 Dafalias, Y.F., "Corotational Rates for Kinematic Hardening at Large Plastic Deformation", *ASME J. Appl. Mech.*, **50**, 561.
- 1983 Franciosi, P., "Glide Mechanisms in BCC Crystals: an Investigation of the case of α -Iron Through Multi-slip and Latent Hardening Tests", *Acta Metall.*, **31**, 1331.
- 1984 Honeycombe, R.W.K., "The Plastic Deformation of Metals". Edward Arnold.
- 1985 Dafalias, Y.F., "The Plastic Spin", *ASME J. Appl. Mech.*, **52**, 865.
- 1985 Havner, K.S., "Comparisons of Crystal Hardening Laws in Multiple Slip", *Int. J. Plasticity*, **1**, 111.
- 1985 Kocks, U.F., "Dislocation Interactions: Flow Stress and Strain Hardening", *Dislocations and Properties of Real Materials*. Institute of Metals, London.
- 1985 Phillips, A. and Das, P.K., "Yield surfaces and Loading Surfaces of Aluminum and Brass: an Experimental Investigation at room and Elevated Temperature", *Int. J. Plasticity*, **1**, 89.
- 1985 Stout, M.G., Martin, P.L., Helling, D.E. and Canova, G.R., "Multi-axial Yield Behavior of 1100 Aluminum Following Various Magnitudes of Prestrain", *Int. J. Plasticity*, **1**, 163.
- 1986 Chaboche, J.L., "Time-Independent Constitutive Theories for Cyclic Plasticity", *Int. J. Plasticity*, **2**, 149.

- 1986 Khan, A.S. and Parikh, Y., "Large Deformation in Polycrystalline Copper under Combined Tension-torsion Loading, Unloading and Reloading or Reverse Loading: a Study of Two Incremental Theories of Plasticity", *Int. J. Plasticity*, **2**, 379.
- 1987 Aifantis, E.C., "The Physics of Plastic Deformation", *Int. J. Plasticity*, **3**, 211.
- 1987 Weng, G.J., "Anisotropic Hardening in Single Crystals and the Plasticity of Polycrystals", *Int. J. Plasticity*, **3**, 315.
- 1987 Weng, G.J., "Anisotropic Hardening in Single Crystals and the Plasticity of Polycrystals", *Int. J. Plasticity*, **3**, 315.
- 1988 Khan, A. and Wang, X., "On Non-proportional Infinitesimal Plastic Deformation After Finite Plastic Prestraining and Partial Unloading", *J. Mech. Phys. Solids*, **36**, 519.
- 1990 Bassani, J.L., "Single Crystal Hardening", *Appl. Mech. Review*, **43**, 320.
- 1990 Dafalias, Y.F. and Aifantis, E.C., "On the Microscopic Origin of the Plastic Spin", *Acta Mech.*, **82**, 31.
- 1990 Khan, A.S. and Wang, X., "An Experimental Study of Large Finite Plastic Deformation in Annealed 1100 Aluminum during Proportional and Non-proportional Biaxial Compression", *Int. J. Plasticity*, **6**, 485.
- 1992 Havner, K.S., "Finite Plastic Deformation of Crystalline Solids". Cambridge University Press.
- 1993 Liang, N.G. and Cheng, P., "A Constitutive Model of Elasto-Plastic Materials Based on Fiber-Reinforcing and Sliding Mechanism", *Science in China*, **36**, 693.