

The Dislocation Moment Field in Polycrystalline Materials

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Continuum description of polycrystalline material is developed on the basis of the continuous dislocation theory. The state of each grain is characterized by the dislocation moments, which are taken as field variables. Physical and mathematical interpretations of the dislocation moments are discussed, and the relation between the plastic strain of the grain and the dislocation configuration in it is studied in detail. The meaning of approximation procedure is also discussed. Stress and energy expressions are considered in terms of the elastic displacement and the dislocation moments. It is shown that our treatment enables us to consider any higher order effects of plastic deformation and that it is reduced to the usual slip theory, if the first approximation is taken.

I. INTRODUCTION

There have been many works on the plastic behavior of polycrystalline materials. The main concern of these works is the slip mechanism of a typical crystal grain of the material, which is assumed to have a single crystalline structure. One of the earliest works is due to Taylor and Elam¹⁾ and developed by Bishop and Hill.²⁾ According to their model, the slip begins along one of a certain set of slip planes, which is determined by the crystal structure of the grain, if the resolved shear stress on the corresponding slip plane exceeds the value of the critical stress. Budiansky *et al.*³⁾ made calculations based on Eshelby's⁴⁾ method of elastic inclusion. Lin and Ito⁵⁾ extended the theory of elasticity to include the crystal slips in the grains.

Meanwhile, it has been known that the crystal slips is caused by means of the dislocation motion. Hence, the plastic behavior must be studied also in terms of the dislocation theory. We are, however, not interested in the details of an individual dislocation line. Rather, we want to know the macroscopic behavior of the aggregate of dislocations. Kröner⁶⁾ developed the theory of continuous dislocation field, and calculated the strain and the stress in terms of given dislocation distribution. Most of his theory, however, concerns uniform single crystalline materials. In polycrystalline materials the dislocation is localized in each of the grains, and there has been no suitable theory so far that takes into account the localization of the continuous dislocation field.

In this work we will show that the continuous field theory of polycrystalline materials based on the continuous dislocation theory is possible, if we consider the *moment* that the dislocation field produces in each grain. We will examine the geometric and physical properties of the dislocation moment and make clear the relation between it and the plastic strain. We will also calculate the stress and the energy in terms of the dislocation moment. Then it will be shown that the phenomenological slip theory is nothing but the first approxima-

tion of our theory. Thus our formulation enables us to study the higher order effects of plastic deformation which are usually ignored in the slip theory.

II. DISLOCATION IN THE GRAIN AND ITS CHARACTERIZATION

In the continuous dislocation theory^{6,7)} the distribution of the dislocation in the material is described by a tensor field a^{ji} , which is called the *dislocation density*. It represents the number of those dislocation lines perpendicular to the unit surface element with its normal along the j -direction that have the unit Burgers vector along the i -direction. It is easily shown that the field a^{ji} is of *no divergence*, i.e.,

$$\partial_j a^{ji} = 0, \quad (1)$$

where ∂_j denotes $\partial/\partial x^j$ and the summation convention is in use. (Our coordinate system is always the orthonormal Cartesian system.)

The motion of the dislocation field is expressed by a tensor field I_j^i , which is called the *dislocation flow*. The time change of the dislocation density a^{ji} is expressed in terms of the dislocation flow I_j^i as follows:

$$\frac{\partial a^{ji}}{\partial t} = \varepsilon^{lkj} \partial_l I_k^i, \quad (2)$$

where ε^{lkj} is Eddington's epsilon which takes the sign of the permutation (lkj) of (123). It has been found that if one looks on the plastic material as a non-Riemannian space, introducing an affine connection into it, the relations (1) and (2) are directly related to the geometric structure of the space-time.^{8,9)} In fact they are interpreted as so called Bianchi's identities. We do not, however, go into these considerations in this paper.

Now let us investigate the dislocation field confined in a particular grain, which we denote by U . We assume that the dislocation does not flow through the surface ∂U of the grain U . Generally speaking, all the properties of the grain depend on the dislocation field a^{ji} in the grain, and the physical quantities such as strain and energy of the grain are *functionals* of a^{ji} . However, if we want to describe the macroscopic behavior of the polycrystalline materials, we must replace these functionals with corresponding *functions* of the quantities that represent the dislocation distribution in the grain as a whole. The simplest of these quantities is of course the total amount of the dislocation in the grain

$$\int_U a^{ji} dV.$$

Let us examine the time derivative of this quantity. Then we see from (2), using Gauss' theorem,

$$\frac{d}{dt} \int_U a^{ji} dV = \varepsilon^{lkj} \int_U \partial_l I_k^i dV = \varepsilon^{lkj} \int_{\partial U} I_k^i dS_l = 0, \quad (3)$$

because we have assumed that there is no dislocation flow through the boundary ∂U of U . Thus, if the material was at first perfect crystal, and the imperfection took place inside the region U , then we obtain the relation.

$$\int_U a^{ji} dV = 0. \quad (4)$$

This result is easily understood, if one recalls the well known crystallographic fact that the dislocation lines are always closed, *i.e.*, they appear as dislocation loops, if they do not pass through the boundary.

III. DISLOCATION MOMENT OF THE GRAIN

Now we must take a further step. Since the crudest of the quantities that characterize the dislocation distribution in the grain is not the total amount of the dislocation, as we have seen, we must consider the amount of *polarization* of it

$$A^{kji} = \frac{1}{|U|} \int_U r^k a^{ji} dV, \quad (5)$$

where r^k is the position vector and $|U|$ is the volume of the grain. We can see from (4) that A^{kji} does not depend on the position of the origin of r^k .

Let us take the time derivative of A^{kji} . Then we obtain, using (2), integrating it by parts, and recalling that there is no dislocation flow through the boundary,

$$\frac{dA^{kji}}{dt} = \frac{\varepsilon^{jml}}{|U|} \int_U r^k \partial_m I_l^i dV = \frac{\varepsilon^{kjl}}{|U|} \int_U I_l^i dV. \quad (6)$$

We always assume that the initial state of the grain is perfect crystal, and therefore A^{kji} vanishes at first. Then we see from (6) the antisymmetry

$$A^{kji} = -A^{jki}, \quad (7)$$

and hence we can reduce the indices by defining

$$A_j^i = \frac{1}{2} \varepsilon_{jlk} A^{lki}. \quad (8)$$

Then (6) takes a simple form

$$\frac{dA_j^i}{dt} = \frac{1}{|U|} \int_U I_j^i dV. \quad (9)$$

We call the quantity A^{kji} (or A_j^i) the *dislocation moment* (of the first order) of the grain.

In order to see the physical meaning of the dislocation moment, let us calculate A_j^i , when there is a single dislocation loop with the Burgers vector b^i (Fig. 1). We obtain, using Stokes' theorem,

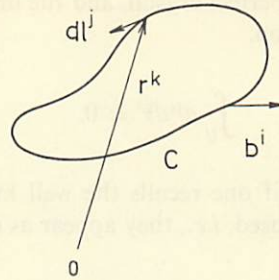


Fig. 1. A dislocation loop with the Burgers vector b^i .

$$A^{kji} = \frac{1}{|U|} \int_C r^k b^i dl^j = \frac{\varepsilon^{kjm}}{|U|} b^i \int dS_m$$

$$\therefore A_j^i = \frac{1}{|U|} S_j b^i, \quad (10)$$

where S_j is the area of the enclosed surface projected on the j -plane. We deduce from this result the following physical interpretation of the dislocation moment.

Proposition 1.

The dislocation moment A_j^i represents the total area of the dislocation loops on the planes with their normals in the j -direction that have the unit Burgers vector in the i -direction.

Then (9) shows the following physical interpretation of the quantity I_j^i .

Proposition 2.

The quantity I_j^i represents the density of the dislocation source (e.g., the Frank-Reed source) which emits the dislocation loops on the plane perpendicular to the j -direction with the unit Burgers vector along the i -direction.

IV. DISLOCATION MOMENTS AND PLASTIC STRAIN

Suppose that the dislocation moment A_j^i of the grain changes its value infinitesimally to $A_j^i + \delta A_j^i$. This change is thought of as caused either by the increase of the area swept by the dislocation lines or by the increase of the Burgers vector, i.e., the simultaneous increase of the slips. In either case the work done by the stress σ^{ji} per unit volume of the grain is

$$\delta W = \sigma^{ji} \delta A_j^i, \quad (11)$$

if the stress is uniform. (Since our coordinate system is Cartesian, we do not make any distinction between upper indices and lower ones.) If all the dislocation loops are caused by single slips, then the Burgers vector b^i of each loop is perpendicular to the normal of the slip plane, and therefore from (10) we see

$$A_i^i = 0. \quad (12)$$

The relation (11) and (12) suggest that the dislocation moment A_j^i is identical to the plastic strain e_{ji} of the grain. To see this, let us cut out from the material a cube with the side length d which contains N dislocation loops with the Burgers vector b as in Fig. 2. Then the plastic strain due to the dislocation is

$$e_{12} = \frac{1}{2} \frac{Nb}{d} = \frac{1}{d^3} \left(\frac{1}{2} d^2 Nb \right) = \frac{1}{2} A_{12}.$$

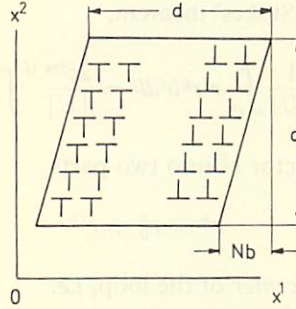


Fig. 2. $A_2^1 > 0$. $A_j^i = 0$, otherwise.

Now we can conclude from this example that the plastic strain e_{ji} is

$$e_{ji} = A_{(ji)}, \quad (13)$$

where () denotes the symmetric part of the components. (We will later give a more general mathematical treatment.) Then (11) and (12) are written as

$$\delta W = \sigma^{ji} \delta e_{ji} \quad (11')$$

$$e_{ii} = 0, \quad (12')$$

as are expected. Moreover, we can see that the antisymmetric part of A_{ji} is the plastic rotation ω_{ji} of the grain:

$$\omega_{ji} = A_{[ji]}. \quad (14)$$

Thus the dislocation moment A_j^i has all the information about the grain deformation to the first order, which is taken into consideration in the usual slip theory.

V. DISLOCATION MOMENTS OF HIGHER ORDERS

We have seen that the dislocation moment A_j^i of the first order represents the first order deformation of the grain. Then it is natural to expect that the dislocation moments of higher orders represent the higher order deformation of the grain. Let us consider the moment of the second order

$$A^{lkji} = \frac{1}{|U|} \int_U r^l r^k a^{ji} dV \tag{15}$$

and differentiate it with respect to time. Integrating it by parts, we obtain

$$\frac{dA^{lkji}}{dt} = \frac{\varepsilon^{nmj}}{|U|} \int_U r^l r^k \partial_n I_m^i dV = \frac{2\varepsilon^{jm}}{|U|} \int_U r^l r^k I_m^i dV. \tag{16}$$

Let us also calculate the moment A^{lkji} of a single dislocation loop with the Burgers vector b^i (Fig. 1). We obtain, by Stokes' theorem,

$$A^{lkji} = \frac{1}{|U|} \int_C r^l r^k b^i dl^j = \frac{2\varepsilon^{jm}}{|U|} \int r^l r^k dS_m b^i. \tag{17}$$

If we decompose the position vector r^k into two parts

$$r^k = r_0^k + r'^k \tag{18}$$

so that r_0^k is the position of the center of the loop, *i.e.*

$$\int r^k dS_n = 0,$$

then (17) is reduced to

$$A^{lkji} = \frac{2\varepsilon^{jm(lk)}}{|U|} r_0^i S_m b^i = \frac{2}{|U|} r_0^{(l} A^{k)ji}. \tag{19}$$

Thus we can think of A^{lkji} as indicating the central position of the loop weighted by its area and the amount of the slip. Hence, generally speaking, the moment A^{lkji} represents the deviation of the distribution of the dislocation loops. Let us take the origin of r^k at the center of the grain. Figure 3 shows the deformation of a cut out material piece such that $A_j^i = 0$ but $A^{lkji} \neq 0$. We can see that A^{lkji} expresses the second order deformation of the grain. Generally we can regard higher order moments A^{lkji} , A^{mlkji} , *etc.*, which are similarly defined, as indicating the higher order deformation of the grain

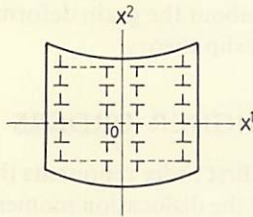


Fig. 3a. $A^{1131} = -A^{3111} = -A^{1311} > 0$.
 $A^{lkji} = 0$, otherwise.

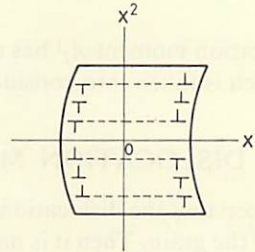


Fig. 3b. $A^{2311} = A^{3211} = -A^{2131} = -A^{1231} > 0$. $A^{lkji} = 0$, otherwise.

VI. APPROXIMATION PROCEDURE OF THE GRAIN DEFORMATION

In this section we study more generally the results intuitively obtained in the previous sections. Let us first consider the dislocation moments A^{kji} and A^{lkji} from the viewpoint of approximation of the function $a^{ji}(\mathbf{r})$.

Suppose we are to approximate the function $a^{ji}(\mathbf{r})$ by a second order polynomial

$$a^{ji}(\mathbf{r}) \cong \overset{0}{a}{}^{ji} + \overset{1}{a}_k{}^{ji}r^k + \overset{2}{a}_{lk}{}^{ji}r^l r^k.$$

One might think of taking the Taylor expansion series. It is, however, not suitable, because the Taylor expansion has the heaviest weight at the origin, while we are interested in the average behavior of $a^{ji}(\mathbf{r})$ in the grain. The approximation should be done not by differentiation. Thus we are led to an idea of taking the least square approximation:

$$\int_U (\overset{0}{a}{}^{ji} + \overset{1}{a}_k{}^{ji}r^k + \overset{2}{a}_{lk}{}^{ji}r^l r^k - a^{ji}(\mathbf{r}))^2 dV \rightarrow \min.$$

Then those coefficients in the approximation are expressed in terms of the integral $\int_U r^k a^{ji} dV$ and $\int_U r^l r^k a^{ji} dV$, i.e. the dislocation moments A^{kji} and A^{lkji} . (Note that $\int_U a^{ji} dV = 0$).

If the grain is assumed to be a sphere of radius h with its center at the origin, then the coefficients are determined as follows.

$$\begin{aligned} \overset{0}{a}{}^{ji} &= - (35/4h^2) A^{kkji} \\ \overset{1}{a}_k{}^{ji} &= (5/h^2) A^{kji} \\ \overset{2}{a}_{lk}{}^{ji} &= (35/2h^4) (A^{lkji} + \frac{1}{2} \delta_{lk} A^{mmji}) \end{aligned} \quad (20)$$

Let F_j^i be the deformation tensor of the material (i.e., an infinitesimally small material piece δx^i in the unstrained state corresponds to $\delta x^i + \delta x^j F_j^i$ in the strained state). Then it is known in the theory of continuous dislocation^{9,10}) that

$$\partial_t F_j^i = \partial_j v^i - I_j^i, \quad (21)$$

where v^i is the velocity field. The relation (21) states that I_j^i is the internal relaxation of the macroscopic deformation $\partial_j v^i$. Now we define the *equivalent velocity* \bar{v}^i by

$$\partial_j \bar{v}^i = I_j^i. \quad (22)$$

(Of course \bar{v}^i may not be determined as a single valued function, but, as will be seen, we need not solve this for \bar{v}^i . We are interested not in a global description but in a point-wise one.) Then the deformation caused by I_j^i and that caused by the corresponding equivalent velocity field \bar{v}_j are equivalent as long as we consider the deformation F_j^i .

Next we consider the grain average of the dislocation flow I_j^i . Let us approximate $I_j^i(\mathbf{r})$ by the linear form

$$I_j^i(\mathbf{r}) \cong \overset{0}{I}_j^i + \overset{1}{I}_{kj}^i r^k \quad (23)$$

in the sense of the least square error. Suppose that the grain is a sphere of radius h whose center is at the origin. Then the coefficients are determined as follows:

$$\begin{aligned} \overset{0}{I}_j^i &= \frac{1}{|U|} \int_U I_j^i dV \\ \overset{1}{I}_{kj}^i &= \frac{1/5h^2}{|U|} \int_U r_k I_j^i dV \end{aligned} \quad (24)$$

Now (9) and (16) are written respectively as

$$\begin{aligned} \frac{dA_j^i}{dt} &= \overset{0}{I}_j^i \\ \frac{dA^{lkji}}{dt} &= 10h^2 \varepsilon_{jkm} (\overset{1}{I}_k)_m^i. \end{aligned} \quad (25)$$

In view of (22), we can think of $\overset{0}{I}_j^i$ and $\overset{1}{I}_{kj}^i$ as the average quantities of $\partial_j \bar{v}^i$ and $\partial_k \partial_j \bar{v}^i$ respectively in the grain. If we introduce the *equivalent displacement* \tilde{u}^i corresponding to the equivalent velocity \bar{v}^i , then (25) implies

$$\begin{aligned} A_{ji} &= \partial_j \tilde{u}_i \\ A_{lkji} &= 10h^2 \varepsilon_{jkm} (\partial_k) \partial_m \tilde{u}^i. \end{aligned} \quad (26)$$

The first of (26) states that the grain with the dislocation moment A_{ji} suffers plastic deformation equivalent to $\partial_j \tilde{u}_i$. This result completely agrees with the consideration in section 4. The expressions (13) and (14) are now written as

$$\begin{aligned} e_{ji} &= \partial_{[j} \tilde{u}_{i]} \\ \omega_{ji} &= \partial_{[j} \tilde{u}_{i]}. \end{aligned} \quad (27)$$

Let us examine the equivalent displacement \tilde{u}_i of the example given in Fig. 3a by using (26). Then we see

$$\begin{aligned} A^{1131} &= -A^{3111} = -10h^2 \partial_1 \partial_2 \tilde{u}_1 > 0 \\ \therefore \partial_1 \partial_2 \tilde{u}_1 &< 0, \end{aligned}$$

which agrees with our previous consideration.

VII. STRESS CAUSED BY THE DISLOCATION MOMENTS

Let us calculate the stress caused by the dislocation moments in the grain. As is known in the theory of elasticity, the stress is determined by means of the stress function χ_{ji} :

$$\sigma^{ji} = - \epsilon^{jlk} \epsilon^{inm} \partial_l \partial_n \chi_{mk} \tag{28}$$

According to Kröner,⁶⁾ the stress function is given in an infinite medium in the form

$$\begin{aligned} \chi_{ik}(\mathbf{r}) &= - \frac{\mu}{4\pi} F_{lkji} \int \eta_{ji}(\mathbf{r}') |\mathbf{r} - \mathbf{r}'| d\mathbf{r}' \\ F_{lkji} &= \delta_{lj} \delta_{ki} + \frac{\nu}{1 - \nu} \delta_{lk} \delta_{ji}, \end{aligned} \tag{29}$$

where η_{ji} is the incompatibility tensor and μ and ν are the rigidity and Poisson's ratio respectively. Since the incompatibility η_{ji} is expressed by the dislocation density a^{ji} in the form

$$\eta_{ji} = 2\epsilon_{ljk} \partial_l a_{ik}, \tag{30}$$

we can obtain, substituting (30) into (29) and integrating it by parts, the following expression.

$$\begin{aligned} \chi_{ml}(\mathbf{r}) &= - \frac{\mu}{2\pi} H_{mlkji} \int a^{ji}(\mathbf{r}') \partial_k |\mathbf{r} - \mathbf{r}'| d\mathbf{r}' \\ H_{mlkji} &= \delta_{j(m\epsilon_l)ki} - \frac{\nu}{1 - \nu} \delta_{ml} \epsilon_{kji} \end{aligned} \tag{31}$$

We assume that the dislocation is confined in a grain whose center is at the origin. If the grain is small compared to \mathbf{r} , then we can develop $|\mathbf{r} - \mathbf{r}'|$ into the Taylor expansion (Fig. 4).

$$|\mathbf{r} - \mathbf{r}'| = r - (\partial_k r) r^{k'} + \frac{1}{2} (\partial_i \partial_k r) r^{i'} r^{k'} + \dots,$$

where $r = |\mathbf{r}|$. Then

$$\frac{1}{|U|} \int_U a^{ji}(\mathbf{r}') |\mathbf{r} - \mathbf{r}'| d\mathbf{r}' = - (\partial_k r) A^{kji} + \frac{1}{2} (\partial_i \partial_k r) A^{lkji} + \dots \tag{32}$$

Hence,

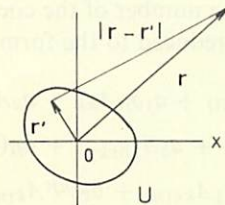


Fig. 4. Dislocations are confined in the grain U.

$$\begin{aligned}\chi_{ml} &= \frac{\mu|U|}{2\pi} H_{mlkji} ((\partial_k \partial_n r) A^{nji} - \frac{1}{2} (\partial_k \partial_q \partial_p r) A^{qpji} + \dots) \\ \partial_k \partial_n r &= \frac{1}{r} \delta_{kn} - \frac{1}{r^3} r_k r_n \\ \partial_k \partial_q \partial_p r &= -\frac{3}{r^3} r_{(k} \delta_{qp)} + \frac{3}{r^5} r_k r_q r_p\end{aligned}\quad (33)$$

If we neglect A^{qpji} and other higher order moments, this expression agrees with that derived by elastic inclusion.⁴⁾ The dislocation moment thus plays an important role, when higher order effects are involved.

If the imperfection is distributed all over the body, then these expressions must be integrated over the body. But this process is tedious. Instead we will consider in the next section a kind of self-consistent approach by extending the self-consistent slip theory.³⁾

VIII. ENERGY AND CONSTITUTIVE EQUATIONS

Let us consider the stored elastic energy of the material, for it plays a fundamental role in the mechanics of continuum. For us it is sufficient only to consider its variational form. We take the macroscopic displacement u_i and the dislocation moments A_{ji} and A_{lkji} as continuous field variables. Since the dislocation moments represent internal relaxation of the strain in the grain, as we saw in section 6, we can deduce from (26) that the increment of the energy takes the form

$$\begin{aligned}\delta U &= \int \sum^{ji} \delta(\partial_j u_i - A_{ji}) dV \\ &+ \int \sum^{lkji} \delta(10h^2 \varepsilon_{jlm} (\partial_k) \partial_m u_i - A_{lkji}) dV.\end{aligned}\quad (34)$$

Now let us consider the constitutive equations of \sum^{ji} and \sum^{lkji} . For simplicity, we assume linearity with respect to A_{ji} , A_{lkji} , $\partial_j u_i$, etc. Moreover, we demand that if there is no plastic imperfection, i.e., $A_{ji} = 0$ and $A_{lkji} = 0$, the energy form be reduced to that of elasticity. We further demand that if the plastic imperfection is of the first order, i.e. $A_{lkji} = 0$, then the form be that of the slip theory. Hence, we can write

$$\begin{aligned}\sum^{lk} &= E^{lkji} \partial_j u_i + F^{lkji} A_{ji} + G^{lknmji} A_{nmji} \\ \sum^{lkji} &= H^{lkjinmqp} A_{nmqp}.\end{aligned}\quad (35)$$

If isotropy is further assumed, the number of the coefficients decreases considerably. For example, the expression of \sum^{lk} is reduced to the form

$$\begin{aligned}\sum^{(ji)} &= \sigma^{ji} + a_0 A_{(ji)} + a_1 \delta_{ji} A_{kk} + a_2 A_{(ji)kk} + a_3 A_{kk(ji)} \\ &+ a_4 A_{k(ji)k} + a_5 A_{(j)kk(i)} + \delta_{ji} (a_6 A_{llkk} + a_7 A_{lkk l}) \\ \sum^{[jil]} &= b_0 A_{[jil]} + b_1 A_{kk[jil]} + b_2 \varepsilon^{kji} A_{k[lnm]l} + b_3 A_{[j]kk(i)} + b_4 A_{k[ij]l} \\ (\sigma^{ji} &= 2\mu \partial_{(j} u_{i)} + \lambda \delta_{ji} \partial_k u_k).\end{aligned}\quad (36)$$

The constants a_0 and a_1 are those determinable by the method of elastic inclusion. According to Eshelby,⁴⁾ they are

$$a_0 = \frac{2\mu}{15} \frac{7 - 5\nu}{1 - \nu}, \quad a_1 = \frac{2\lambda}{3} \frac{1 - 2\nu}{1 - \nu}. \quad (37)$$

IX. CONCLUSION

We intended to develop a continuum theory of polycrystalline materials, characterizing the state of each grain by the dislocation moment, and we have so far investigated various properties of the dislocation moment and the role it plays in the mechanics of polycrystalline materials. In order to calculate the details of plastic behavior, we must give a suitable yield condition of the material. The detailed analysis is beyond the range of this paper. However, we should note that if we restrict our attention to the first order dislocation moment, our theory is reduced to the phenomenological slip theory. Since we take a structural point of view in the sense that our formulation is based on consideration of the dislocation configuration in the grain, the author believes that this approach will enable us to obtain solutions of various plastic behavior with higher accuracy.

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