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Elastic Deformation of Polycrystalline Metal*

(1st Report, Influence of grain shape on distributions of stress and strain in grains)

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Stress and strain distributions in polycrystalline aggregates during uniaxial elastic deformation were investigated adopting the finite element method. The effect of grain shape on the deformation mode was studied. The distribution of the constraint ratio between grains defined previously was calculated for each grain shape.

It was found that the strain is continuous across the grain boundary parallel to the stress axis, while the stress is continuous across the grain boundary perpendicular or inclined to the stress axis.

The deformation of island grains was also discussed.

1. Introduction

Metals used for structural members or machine parts are polycrystalline. So, it is necessary to discuss the deformation or fracture of metals from the view point of polycrystalline aggregates. It is the purpose of the present series of studies to clarify the basic characteristics of the deformation of polycrystalline metal.

In the previous reports⁽¹⁾⁽²⁾, the deformation of polycrystalline metal was discussed from the stand point of energy assuming that the polycrystals are composed of discontinuous media. In the course of the study, it has become necessary to know the distributions of stress and strain in a grain quantitatively. In the present paper, therefore, the deformation of polycrystalline metal which has discontinuous boundary is investigated from the view point of continuum mechanics.

It is considered that the distributions of stress and strain in a grain play an important role in elastic or plastic deformation of polycrystalline metals. In most of the previous articles on analytical studies of crystal plasticity, the distributions of stress and strain in grains are scarcely discussed.

The distributions of stress and strain in a grain are caused by the anisotropy of crystal. Generally, the anisotropy of crystal related to the strength of metal is composed of four factors.

- (1) Anisotropy of elastic constants
- (2) Anisotropy of yielding

- (3) Anisotropy of work-hardening
- (4) Anisotropy of fracture

Two methods, the analytical method and experimental one, may be available to obtain the distributions of stress and strain in a grain caused by those anisotropies. The analytical method is further divided into the following two types.

- (a) Analysis of materials with discontinuous boundary by means of continuum mechanics
- (b) Analysis based on the crystallographic conditions such as slip plane and so on.

In the present report, the distributions of stress and strain in grains after elastic deformation are calculated from the stand-point of (a) with the finite element method. The applied stress is supposed to be uniaxial. It seems, however, necessary here to make clear the basic correlation of the present analytical study with the anisotropy of crystal, before the process of the analysis is described in detail.

From the crystallographic point of view, the elastic anisotropy of crystal is defined by the three elastic constants or elastic compliances s_{11} , s_{12} and s_{44} ⁽³⁾ for a cubic crystal (most metals used as structural members have the cubic crystallographic structure). When the crystal axes coincide with the stress axes, the strains are given by

$$\epsilon_1 = s_{11}\sigma_1, \quad \epsilon_2 = \epsilon_3 = s_{12}\sigma_1 \dots\dots\dots (1)$$

where σ_1 is the applied uniaxial stress. Generally, if the stress axes are expressed by x - y - z coordinates, the strains are given by⁽⁴⁾,

$$\left. \begin{aligned} \epsilon_x &= s_{11}'\sigma_x, & s_{11}' &= s_{11} - 2\lambda P \\ \epsilon_y &= (s_{12}')_y\sigma_x, & (s_{12}')_y &= s_{12} + \lambda Q_y \\ \epsilon_z &= (s_{12}')_z\sigma_x, & (s_{12}')_z &= s_{12} + \lambda Q_z \\ \lambda &= s_{11} - s_{12} - s_{44}/2 \end{aligned} \right\} \dots\dots\dots (2)$$

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where P , Q_y and Q_z are the coefficients determined independently by the mutual relation of the orientation between the stress axes and the crystal axes.

On the other hand, in the theory of isotropic elasticity, the difference in elastic constant between grains is usually defined by the differences in Young's modulus E and Poisson's ratio ν , which are correlated to the above crystal anisotropy in the following way.

$$s_{11}' = \frac{1}{E}, \quad (s_{12}')_y = (s_{12}')_z = -\frac{\nu}{E} \dots \dots \dots (3)$$

s_{11}' and s_{12}' change independently according to the orientation of grains and so do E and ν .

Therefore, it is necessary to separate the effects of Young's modulus E and Poisson's ratio ν , to clarify the influence of anisotropy.

In the present report, the main focus is put on the effect of Young's modulus E , which is expected to be most effective. Poisson's ratio ν is assumed to be constant in the polycrystals (the influence of the anisotropy of Poisson's ratio will be reported elsewhere). The purpose of the present report is to propose simplified models of polycrystals composed of grains having the anisotropy of elastic constant and to clarify the basic behavior of the deformation of anisotropic materials.

The constraint ratio defined in the previous paper⁽¹⁾ is used to denote the mode of deformation quantitatively. Discussions are made to clarify the effects of the grain shape, the inclination angle of the grain boundary to the stress axis, the difference in Young's modulus between the neighboring grains, Poisson's ratio of the polycrystals, the mean strain, etc., on the mode of deformation, namely, the distributions of stress, strain and constraint ratio in the polycrystals.

In the following, grains in polycrystalline metal are approximated to simple geometrical models. Although it may be necessary to analyse the deformation three-dimensionally for comparison of the analytical result of it with the deformation behavior of practical metals, it is rather complicated. So, two-dimensional analysis was used in the present report, and two basic problems, (1) basic mechanical properties of discontinuous boundary and (2) factors affecting the constraint at grain boundary, are studied. This is done based on the idea that the effect of grain boundary is represented in the first approximation by a change in the plane perpendicular to the grain boundary containing the stress axis, though the configuration of grains in polycrystals is three-dimensional.

2. Analysis

At first, a square model of polycrystalline metal shown in Fig. 1(a) is considered. Two sorts of grains having Young's modulus $E_1 (E_1 < E_0)$ and

$E_2 (E_2 > E_0)$ lie reciprocally as shown in the figure. E_0 is the mean value of Young's modulus. The two sorts of grains are expressed with the signs $-$ and $+$ respectively in the figure. Owing to the symmetry of the configuration of grains, it is sufficient that the stress or the strain be calculated in the square OACB surrounded with the broken line in Fig. 1(a), as representative of the whole polycrystal. Each side of the square remains straight after deformation. The square changes its shape into rectangular. The stress and the strain distributions are calculated in the square OACB as shown in Fig. 1(b). Young's modulus of the grains are expressed by

$$\frac{1}{E_1} = \frac{1}{E_0}(1+\varphi), \quad \frac{1}{E_2} = \frac{1}{E_0}(1-\varphi) \dots \dots \dots (4)$$

where φ is a parameter corresponding to the difference in Young's modulus in both grains. E_0 is equivalent to the mean Young's modulus $\bar{E}_s$ under the condition of constant stress. When the finite element method is used, it is possible to calculate those grains which have a relatively large difference in Young's modulus. To show the distributions of stress and strain clearly, a large difference in Young's

modulus i.e., $\varphi=0.8(E_2/E_1=9)$ is mostly used. The effect of the parameter φ of anisotropy on the results is also discussed.

The finite element method is very useful for the analysis of continua if a computer with large core memory is used⁽⁵⁾. The displacement method is adopted in the calculation of the finite element method. As a boundary condition, the side line BC in Fig. 1(b) is assumed to move in the direction of the stress axis by a unit displacement, and the side line AC moves in the perpendicular direction to the stress axis by $-\nu$, where ν is Poisson's ratio. ν is mostly taken to be 0.3 in the following calculation. It is a characteristic of the finite element method that the boundary condition is given by the displacement.

Let us denote the total stiffness matrix, the load matrix and the displacement matrix by $[K]$, $[P]$ and $[d]$, respectively. The displacement matrix $[d]$ is divided into two parts, one being the known displacement $[d_S]$ of the nodes on the boundary, and the other the unknown displacement $[d_F]$ of the other nodes⁽⁶⁾.

$$\begin{bmatrix} K_{FF} & K_{FS} \\ K_{SF} & K_{SS} \end{bmatrix} \begin{bmatrix} d_F \\ d_S \end{bmatrix} = \begin{bmatrix} P_F \\ P_S \end{bmatrix} \quad (5)$$

The applied force acts only on the node on the boundary, and then in the present case $[P_F]=[0]$. Therefore, from Eq. (5) we have

$$[K_{FF}][d_F] = -[K_{FS}][d_S] \quad (6)$$

Equation (6) can be solved as simultaneous equations of the first order, for the right side of the equation is known. The band method⁽⁷⁾ for the calculation of the equations by computer saves the capacity of core memory and the time for calculation. The triangular elements were used. The numbers of divisions of the elements are both 32 and 128 elements as shown in Fig. 3 or 6 and Fig. 2, respectively. The former is used for the qualitative discussion and the latter for the quantitative discussion.

Fig. 2 An example of divided elements (128 elements)

In the deformation of polycrystals composed of anisotropic crystal, the distributions of stress and strain are greatly affected by the mutual restriction between grains across the grain boundary. The constraint ratio η is defined in the following way⁽¹⁾.

The strain ϵ in an arbitrary grain is expressed by

$$\epsilon = \bar{\epsilon} + \Delta\epsilon \quad (7)$$

where $\bar{\epsilon}$ is the mean value of strain for the polycrystals. Then, the value of constraint ratio in the grain is defined by

$$\eta = \Delta\epsilon / (\Delta\epsilon)_{\max} \quad (8)$$

where $(\Delta\epsilon)_{\max}$ is the value of $\Delta\epsilon$ under the constant stress condition. $\eta=0$ and $\eta=1$ correspond respectively to the conditions of constant strain and constant stress⁽¹⁾. In the practical calculation, the value of η is obtained by the following equation⁽¹⁾⁽²⁾.

$$\eta = \frac{-\bar{E}_\epsilon \Delta\epsilon}{\Delta E_\epsilon \bar{\epsilon}} \quad (9)$$

where $\bar{E}_\epsilon$ is the mean value of Young's modulus under the condition of constant strain, and $E = \bar{E}_\epsilon + \Delta E_\epsilon$.

3. Results and discussions

In the following figures, the calculated distributions of stress, strain and constraint ratios are shown for various shapes of grains. The axial stress σ_x and axial strain ϵ_x are shown in the figures, instead of the principal stress and the principal strain. This is because the purpose of the present study is to clarify the basic feature of the stress and strain near the grain boundary and that the grain shape assumed in the following analysis is only an idealized one and the grain shape and its configuration in real metals are usually more complicated. The values of stress and strain in each element shown in the following figures are the mean values for the element⁽⁵⁾. The units of the stress and the strain are taken arbitrarily in each figure.

Figure 3 shows the axial stress and the axial strain in the region OACB shown in Fig. 1(b). The grain boundary is indicated with a thick line. The length of the line with arrows at the both ends shows the relative value of the stress and the strain. In the central region of the grain, that is, in the regions at the four corners of the square OACB in Fig. 3, the mode of deformation is almost the same as that of constant stress, and the strain is different according to the difference in Young's modulus. The mode of deformation near the grain boundary parallel to the stress axis is different from that perpendicular to the stress axis. The difference in the stress between the grains on the both sides of the grain boundary perpendicular to the stress axis is relatively small, while the difference in the strain is relatively large.

On the other hand, the strain is continuous across the boundary parallel to the stress axis, while the stress is discontinuous.

The changes in stress and strain across the grain boundary parallel to the stress axis are shown quantitatively in Figs. 4 and 5. The solid lines (○ marks) show the distributions of stress, strain and constraint ratio along $x/a=1/16$ and $7/16$, calculated from the

128 divided elements (Fig. 2). The unit of strain is the ratio of the strain to the mean strain $\bar{\epsilon}_x$ which is determined from the boundary condition. Similarly, the unit of stress is the ratio of the stress to the product $\bar{E}_0 \bar{\epsilon}_x$ of the mean elastic constant under the condition of constant stress and the mean strain. Each point (○ marks) represents the mean value of the two opposite triangular elements, which is equal to the value of the corresponding square element.

It can be said from Figs. 4 and 5 that the maximum stress appears near the grain boundary in the grain which has a large value of Young's modulus E_2 . It was reported⁽⁸⁾ from the etch pit observation of the surface that in the pre-yielding region of copper, the initiation of micro-yielding or the multiplication of dislocations starts in the region near the grain boundary. It is considered that the micro-yielding starts preferentially in the above high stressed

Fig. 3 Distributions of stress and strain in square grains

Fig. 4 Distributions of stress, strain and constraint ratio ($\phi=0.8$)

Fig. 5 Distributions of stress, strain and constraint ratio ($\phi=0.8$)

region near the grain boundary.

The plane stress condition ($\sigma_z=0$) or the plane strain condition ($\varepsilon_z=0$) is usually assumed in the two-dimensional analysis of continuum mechanics. The influence of the both assumptions on the calculated mode of deformation was studied and the result is shown in Figs. 4 and 5. The $\circ$ marks represent the

result obtained from the plane stress condition and the $\bullet$ marks the one from the plane strain. It may be concluded from Figs. 4 and 5 that the difference in the distribution of stress, strain or constraint ratio between the conditions of plane stress and plane strain is very small. The mean value $\bar{\eta}$ of constraint ratio for polycrystals is also nearly the same, that is, $\bar{\eta}=0.74$ for the plane stress and $\bar{\eta}=0.75$ for the plane strain (Table 1). In the following, the calculations are made mainly with the condition of plane stress.

The maximum angle between the direction of applied stress and the principal stress is about 20° in the element near the corner of the grain boundary of the 128 divided elements. The angle is relatively small in general and σ_y is much smaller than σ_x .

Based on the above results for the case of $\varphi=0.8$ ($E_2/E_1=9$), the influence of the value of φ or E_2/E_1 on the mode of deformation was investigated. The distributions of stress, strain and constraint ratio along $x/a=1/16$ are shown in Fig. 6 for $\varphi=0.8$, $\varphi=0.4$ ($E_2/E_1 \approx 2.3$) and $\varphi=0.05$ ($E_2/E_1 \approx 1.1$). The distributions of constraint ratio η are almost the same, though the absolute values of stress and strain change with φ . The mean value $\bar{\eta}$ of constraint

Fig. 6 Distributions of stress, strain and constraint ratio

Table 1 Mean value of constraint ratio for polycrystals

	Boundary condition	φ	Poisson's ratio ν	Mean value of constraint ratio $\bar{\eta}$	Remarks
Square grains	Plane stress	0.8	0.3	0.74	Fig. 3
	Plane strain	0.8	0.3	0.75	
	Plane stress	0.4	0.3	0.72	
	"	0.05	0.3	0.72	
	"	0.8	0.35	0.74	
Rhombic grains	"	0.8	0.25	0.73	Fig. 15
	Plane stress	0.8	0.3	0.59	
	"	0.4	0.3	0.56	
	"	0.8	0.25	0.60

Fig. 7 Distributions of stress and strain in grains with triple point of grain boundary

Fig. 8 Model of square island grains

ratio for square grains is 0.72 for the both cases of $\varphi=0.4$ and $\varphi=0.05$ (Table 1). Hereafter, φ is mainly taken as 0.8 to show the trends of the results clearly, which may be applicable to the case of small value of φ .

In the calculation, a constant axial mean strain is given as a boundary condition (in the present calculation the mean strain $\bar{\epsilon}_x$ is 0.003125). No effect of the mean strain has appeared on the de-

formation mode, as far as the stress or the strain is expressed nondimensionally (Fig. 4~6). It may be noteworthy that the distribution of η calculated with the two-dimensional elasticity is not affected by the mean strain $\bar{\epsilon}_x$.

Figure 7 shows the result for grains which have the T-type triple point of grain boundary. The distributions of stress, strain and constraint ratio along the line $x/a=1/16$ and $7/16$ are shown with the broken line (● marks) in Figs. 4 and 5. It is shown that the value of η is smaller for the grains with the triple point of grain boundary, that is, the deformation mode is closer to the condition of constant strain than that of the square grains (○ marks in Figs. 4 and 5). Consequently, it is concluded that the adjacent grain in the stress direction affects the deformation mode of grains and that η increases as the difference of Young's modulus E between the adjacent grains increases. The mode of deformation comes close to the condition of constant strain, as the difference in E decreases.

Next, a model of island grains shown in Fig. 8 is considered, which corresponds to the metals having the second phase or precipitates. The distributions of stress and strain are calculated in the region surrounded with the boundary of the broken line in Fig. 8, considering from the symmetry of the grain configuration. The result for $\varphi=0.8$ is shown in Fig. 9, where Young's modulus of island grains is larger than that of the matrix. Meanwhile, Fig. 10 shows the result for $\varphi=-0.8$, i.e. Young's modulus

Fig. 9 Distributions of stress and strain around square island grain

Fig. 10 Distributions of stress and strain around square island grain.

Fig. 11 Distributions of constraint ratio in materials having square island grain and octagonal island grain

of the island grains is smaller than that of the matrix.

The distributions of η corresponding to the lines

Fig. 12 Distributions of stress and strain around rectangular island grain (The longer axis of grain is parallel to the stress axis)

Fig. 13 Distributions of stress and strain around rectangular island grain (The longer axis of grain is perpendicular to the stress axis)

Fig. 14 Model of polycrystalline aggregates (rhombic grains)

Fig. 15 Distributions of stress and strain in rhombic grains

$x/a=1/32, 9/32$ and $15/32$ in Fig. 9 are calculated and shown with $\circ$ marks in Fig. 11(a), (b) and (c), respectively. The results corresponding to

Fig. 10 are shown with $\bullet$ marks in the same figure. Figure 11 shows that η is large in the region $y/a < 1/2$, η is small constant in the region $y/a > 1/2$. The deformation mode is different according to whether Young's modulus of the island grain is larger than that of the matrix or smaller.

The calculation is also made for the rectangular island grains, one having a long axis in the direction of stress and the other having a long axis in the direction perpendicular to the stress axis. The results are shown in Figs. 12 and 13, respectively. The deformation mode shown in Fig. 12 is nearly equal to the condition of constant strain. Meanwhile, the deformation mode is almost equal to the deformation under the constant stress condition in Fig. 13. The distributions of stress and strain are largely affected by the shape of island grains, which may be due to the ratio of the lengths of grain boundaries between the parallel one to the stress axis and the perpendicular one to it.

Next, in order to consider the polycrystals having inclined grain

boundary to the stress axis, rhombic grains are assumed as representative ones. It is sufficient here again to consider the region shown with the broken line in Fig. 14 by the symmetry of the grain configuration. The result is shown in Fig. 15. Neither the stress nor the strain is constant in the grains. The distributions of constraint ratio along the lines $x/a=3/32$, $7/32$ and $13/32$ in Fig. 15 are shown with $\circ$ marks in Fig. 16(a), (b) and (c), respectively. The value of η is relatively large near the grain boundary, which is similar to the change in η near the grain boundary perpendicular to the stress axis of the square grains. Namely, the stress is rather continuous across the grain boundary compared with the strain. The mean values $\bar{\eta}$ of constraint ratio for the rhombic polycrystals are listed in Table 1 and are seen to be smaller than that of the square grains.

Consequently, the inclination angle of the grain boundary to the stress axis affects the deformation mode of polycrystals.

The result for the case of $\varphi=0.4$ shown with the $\bullet$ marks in Fig. 16 is similar to the case $\varphi=0.8$ ($\circ$ marks). The effect of φ on the distribution of constraint ratio is again very small. As men-

tioned before, the anisotropy of grain under uniaxial stressing is denoted by the differences in Young's modulus E and Poisson's ratio ν . The result for Poisson's ratio $\nu=0.25$ is shown with $\bullet$ marks in Fig. 16. The influence of Poisson's ratio ν on the deformation mode is much smaller than that of Young's modulus. This is also confirmed by the mean value $\bar{\eta}$ of constraint ratio shown in Table 1.

The value of constraint ratio η becomes greater than unity or less than zero in some regions of the grains as shown in Fig. 11 or 16. The mean value $\bar{\epsilon}$ of the strain for the polycrystals is used to calculate the value of η from Eq. (9). So, the fact that the value of η is off the range from 0 to 1 is considered to indicate that the local average strain $\bar{\epsilon}_{\text{local}}$ for the regions is different from the mean strain $\bar{\epsilon}$ for the polycrystals or η represents a kind of stress concentration. There seems to be some sway in the distribution of strain in polycrystals.

Figure 18 shows the result of calculation for the rhombic island grains shown in Fig. 17. Both the stress and the strain change in the grain and the matrix, which is similar to the trend shown in Fig. 15.

Figure 19 shows the distributions of stress and strain for the octagonal island grains. A combined trend

Fig. 16 Distributions of constraint ratio in rhombic grains

Fig. 17 Model of rhombic island grains

Fig. 18 Distributions of stress and strain around rhombic island grain

of the results for the square island grain (Fig. 9) and for the rhombic island grain (Fig. 18) seems to have appeared. The distribution of constraint ratio for the octagonal island grains is shown with $\bullet$ marks in Fig. 11. As is seen from Fig. 11, the distribution of η is smoother than in the case of square island grains ($\circ$ marks). The concentrations of the stress and the strain at the corner of the square island grain seem to be relieved in the case of the octagonal island grains.

The basic feature of the influence of the grain shape on the deformation mode of polycrystals has become clear from the above. Further quantitative discussions may be necessary, which will be reported later.

4. Conclusions

Discussions are made on the elastic deformation of polycrystals under uniaxial stress. Especially, the effects of the shape of grains are discussed with several models of polycrystals, based on the finite element analysis. The results may be summarized as follows.

(1) The deformation of the grain is restricted at the grain boundary parallel to the stress axis. So, the axial strain is continuous at the boundary, while the stress is discontinuous.

(2) On the other hand, at the grain boundary perpendicular to the stress axis, the stress is continuous, while the strain is discontinuous. The deformation mode of grains is also affected by the value of Young's modulus of the adjacent grain in the direction of stress axis.

(3) If the grain boundary is inclined to the stress axis, neither the stress nor the strain is constant in the polycrystals. The stress is comparatively continuous, however, at the grain boundary. The inclination angle of the grain boundary to the stress axis considerably affects the distributions of stress, strain and constraint ratio.

(4) Similar trends are seen for with the island grains which have different values of Young's modulus from the matrix. If the island grain is long in the direction of the stress axis, the mode of

Fig. 19 Distribution of stress and strain around octagonal island grain

deformation is close to the condition of constant strain. On the other hand, if the island grain is long in the perpendicular direction to the stress axis, the mode is close to the condition of constant stress.

(5) The value of the mean axial strain has no effect on the distribution of constraint ratio in the elastic deformation. The distribution of constraint ratio shows little change depending on the magnitude of the difference of Young's modulus between grains.

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References

- (1) Abe, T., *Bull. JSME*, Vol. 12, No. 50 (1969-4), p. 165.
- (2) Abe, T., *Bull. JSME*, Vol. 14, No. 78 (1971-12), p. 1263.
- (3) Kittel, C., *Introduction to Solid State Physics*, (1966), John-Wiley & Sons.
- (4) Takechi H. and Kato, H., *5th X-ray Symposium (Japan)*, (1968), p.3, Society of Materials Science, Japan.
- (5) Zienkiewicz O.C., and Cheung, Y.K., *The Finite Element Method in Structural and Continuum Mechanics*, (1967), McGraw-Hill.
- (6) Sakurai, T., *JSSC (in Japanese)*, Vol. 3, No. 21 (1967), p. 62.
- (7) Weaver, W., *Computer Programs for Structural Analysis*, (1967), Van Nostrand.
- (8) Vellaikal, G., *Acta Met.*, Vol. 17 (1969), p. 1145.

Discussion

R. KOTERAZAWA (Osaka University):

(1) Although the paper is intended to analyse the influence of elastic anisotropy of crystal, the difference between the elastic constant in the longitudinal direction and the one in the transverse direction does not seem to be taken into account in the analysis. So, the model is considered to correspond to elastic non-homogeneity instead of elastic anisotropy.

(2) The author's explanation may be accepted for the deformation under uniaxial stress. But it might not be applicable to the deformation under biaxial stress treated in the present paper. In the paper the elastically anisotropic behavior of polycrystals is deduced from the analysis of the elastically non-homogeneous materials by the finite element method. Although I did not deny that there is some adequacy of the deduction, it seems difficult to declare that the present analysis and results strictly correspond to the materials having elastic anisotropy.

(3) It is mentioned that the case of $\eta > 1$ or $\eta < 0$ corresponds to the fact that η represents a kind of stress concentration and this effect has not been discussed in the field of elastic deformation of polycrystals or crystal plasticity. The problem of the stress concentration in a non-homogeneous material, however, is considered to be fundamentally related to the previous studies such as the stress concentration around inclusions. So, the discussion in the present study should have been made in reference to those previous studies, and then more effective discussions would have been made.

(4) The conclusion that the distribution of η is not dependent on the total strain seems to be self-evident and may be reached without any numerical calculation, as far as the linear elasticity of material is assumed in the analysis. The same thing may be said about the ratio E_1/E_2 ?

(5) If the author's intension is to analyse many factors, those factors whose effects are known without numerical calculation should be separately shown from those which require the calculation by the finite element method, for those two are different in the meaning and the generality from each other.

What is the reason to think that the deformation behavior differs with the ratio E_1/E_2 , in spite of the assumption of linear elasticity of the materials?

(6) It seems that only qualitative discussions are made in the paper, but quantitative relations are most essential in this sort of calculation. I wonder how much influence will appear with the actual polycrystalline metals (or non-homogeneous medium such as metals with inclusions)? The experimental result

on the initial yield in copper is explained by the stress concentration near the grain boundary, but what is the ground for the reasoning that the experimental result is caused only by the factor discussed in the present paper?

Author's closure

(1) Although the present model simplifies the practical polycrystalline metal with some approximations, the basic behavior of polycrystalline is considered to be represented with this model in the following way. When the deformation under uniaxial stress is considered, the longitudinal elastic constant (elastic compliance) is $s_{11}' = 1/E$, and the transverse elastic constant is $s_{12}' = -\nu/E$. So, the difference between the elastic constants in the longitudinal and in the transverse is expressed with Poisson's ratio ν . However, the anisotropy of the transverse elastic constants between y direction and z direction, where the stress axis is taken as x -axis, is not considered in the present study. The effect of the latter anisotropy could be calculated by taking it into consideration in the stiffness matrix of the finite element method, but the effect is expected to be very small as compared with that of the anisotropy of the longitudinal elastic constant.

(2) The applied force is uniaxial in the present analysis. Although the biaxial stress state might be present in the regions near the corner of grain boundary, the rotation of stress axis in the corner triangular element is about 20° and hence the stress in the axial direction is large as compared with that in the transverse direction.

Models of polycrystals are used in the present study to analyse the elastic deformation of polycrystals, where some approximations are made. However, the most effective factor affecting the mode of deformation of polycrystals is considered to be the difference in the axial strains between two grains adjacent in the perpendicular direction to the stress axis, which is caused by the difference in Young's modulus between the two grains. This situation is taken into account in the present model. Therefore, it is considered that the present result expresses the basic characteristics of the deformation behavior of polycrystals. In other words, the present study analyses the modeled anisotropic medium, i.e., the modeled polycrystals.

(3) It is of course necessary to consider the correlation of the present study with the problem of the stress concentration. The author particularly pointed out in the paper that there is some sway in

the distribution of strain in the polycrystals after elastic deformation, which has not been considered in the analytical study of the elastic deformation of polycrystals or crystal plasticity. It is expected, for instance, that the sway of strain results in a roughening of the surface of metals after plastic deformation.

(4) In the field of experimental study of deformation of polycrystals such as lattice strain measured by X-ray, it is a point of controversy whether the mutual restriction between grains is dependent on the total strain or grain size in elastic or plastic deformation or not. Many factors affecting the mode of deformation of polycrystals are listed in the present paper. The fact that the constraint ratio is independent of the total strain is considered to result from the assumed linear elastic nature of materials. It is considered that the behavior of deformation is different with the ratio E_1/E_2 for those elastic media containing discontinuous boundaries of elastic constant respectively inclined to the stress axis. The present calculations are made for a relatively large ratio of Young's modulus, i.e. $E_2/E_1=9$, to show the distribution of stress in grains clearly. Although the ratio is not so large in the practical metals, (ex. $E_{\max}/E_{\min} \cong 2.4$ for iron), it is expected that the result of the present calculation is applicable to practical metals, for the effect of the ratio E_2/E_1 on the result of calculation is relatively small.

(5) Although the description in the main text is slightly insufficient, the fact that the distribution of the constraint ratio η is independent of the total strain was also concluded from the general analysis of polycrystals reported previously⁽¹⁾. It is planned to study the influence of several factors such as the total strain etc. on the mode of deformation of polycrystals after slip of plastic deformation occurs in grains, and compare the result with the result of elastic deformation.

It is not clear at present why the deformation behavior is different with the ratio E_1/E_2 . It is

observed, however, that the averaged strain along the line $x/a=0$ is smaller than the averaged strain along the line $x/a=1/2$, in the case of the rectangular grains whose shape is longer in the direction of stress axis, which is possibly related to the presence of the cross point of grain boundary in the model. (Further results of calculation will be presented in the next report.)

(6) The influence of grain shape on the deformation behavior of polycrystals has not been studied yet, and it seems necessary, first of all, to define the problems in the research. Thus, in the present study, general discussions are made based on the models of polycrystals in which grain boundaries inclined to the stress axis occupy respective portions of the total length of the grain boundary. It is of course necessary to make quantitative discussions on the problems pointed out in the present study. The influence of the ratio of the length of longitudinal grain boundary to that of perpendicular grain boundary in the rectangular grains on mean Young's modulus will be discussed in the second report.

The correlation of the present study with the initial yielding is considered as follows. The shear stress on the slip plane is large near the grain boundary if the axial stress is greater near the grain boundary than in the center of grain. Therefore, if the critical shear stress or the force to activate dislocation sources such as Frank-Reed source is equal in the center of the grain and near the grain boundary, a slip is considered to start near the grain boundary where the stress is high. (In the discussion, it is supposed that the grain boundary itself is not the source of dislocation⁽⁹⁾).

The slip started near the grain boundary was also observed by H. Miyamoto et al.*

* Miyamoto, H., et al., *Int. Conf. on Mech. Behavior of Materials*, Kyoto 1971, Abstract, Vol. 1, p.399.