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Influence of Free Surface on Mutual Restriction between Grains in Elastic Deformation of Polycrystals *

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Elastic deformation of polycrystalline metals under uniaxial loading is investigated by analysing a model of polycrystals by finite element method. Influence of free surface on deformation behavior of grains and three-dimensional restriction of grains are mainly studied.

It was found that the effect of free surface on distribution of stresses, strains or constraint ratios in the stress direction in surface grains is small and confined to a very thin layer near the surface. The stress normal to surface is nearly equal to zero in the surface grain, while the strain or constraint ratio normal to surface changes. There is little effect of free surface on the distribution of stresses, strains and constraint ratios in the inner grains adjacent to the surface grains. Group of grains placed near the surface of polycrystals is found to rotate during deformation.

The distribution of constraint ratios in the stress direction in the surface grains is approximately represented with cosine curve as well as that in the interior grain. It is suggested, however, that the mean constraint ratio in the surface grain is about 75-89 % of that in the interior grain, because grains are cut by surface randomly and hence the depth of the surface grains is random. It is also suggested that three-dimensional restriction is nearly double the two-dimensional one.

1. Introduction

The objective of the present study is to clarify the effect of free surface on elastic deformation of polycrystals analytically. The method of analysis on the restriction between grains in elastic deformation of polycrystals reported previously⁽¹⁾⁻⁽⁴⁾ is applied for this purpose. To know the effect of surface on deformation is important for some application problems, as well as for basic investigation of deformation behavior of materials. For instance, it was pointed out⁽⁵⁾ that the value of constraint ratio near the surface of specimen is necessary to obtain X-ray elastic constant analytically, which is used in X-ray stress measurement, for the penetration depth of X-ray into metals is very small. As another example, surface roughening is known as one of important problems in getting precise and fine products in plastic metal working process. The surface roughening is essentially caused by plastic anisotropy or non-uniform plastic deformation of metals. Discussion on the influence of free surface on elastic deformation of polycrystals will give basis for the further study on plastic deformation.

Some analyses have been done on surface mechanics⁽⁶⁾, but no analytical study seems to have been made on the

effect of surface on deformation behavior of polycrystals.

The previous discussions⁽¹⁾⁻⁽⁸⁾ were based on the calculated results with a plane model of polycrystals. It is necessary in general, however, to analyse three-dimensional restriction of grains, especially to consider the influence of free surface.

Therefore, the following two points are mainly studied in the present paper; (1) Influence of free surface on deformation behavior of grains, and (2) three-dimensional restriction of grains.

The applied load is assumed to be uniaxial in the following.

2. Influence of surface

The distribution of constraint ratios near the surface is calculated at first, with a plane model of polycrystals and finite element analysis. Rectangular coordinates (x, y, z) is used, where x and z axes are in the stress direction and in the normal direction to surface, respectively.

2. 1. Model of polycrystals

The plane model of polycrystals shown in Fig. 1(b) is used to calculate stress, strain and constraint ratio (which was introduced⁽¹⁾⁻⁽⁴⁾ to represent restriction of grains qualitatively) in the grains near the surface of polycrystals. The first and the second layer grains are named hereafter the surface grains and the inner grains, respectively, as shown in Fig. 2. Fig. 1(a) is a model of bulk polycrystals which is named the interior

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grains in the following. It is assumed⁽¹⁾⁻⁽³⁾ in both models that two kinds of grains having different values of Young's modulus lie alternately, which are shown with the marks + and -, respectively, in Fig. 1. The values of Young's modulus for the respective grains are assumed to be expressed as follows with a parameter ϕ of anisotropy^(*).

$$E_1 = \bar{E}_s(1+\phi), \quad E_2 = \bar{E}_s(1-\phi) \dots \dots \dots (1)$$

where $\bar{E}_s$ is the mean value of Young's modulus under constant strain condition (Voigt model of deformation) (the upper wavy line represents mean value for polycrystals). It is possible to choose the representative area OACB in Fig. 1 for the following calculation, owing to the symmetric configuration of grains⁽¹⁾.

The aspect ratio of the interior grains is denoted by⁽²⁾

$$R = b/a \dots \dots \dots (2)$$

where a and b are the longitudinal length and the width of grain, respectively (c.f. Fig. 2). Similarly, the aspect ratio R' of surface grain is defined by

$$R' = 2b'/b \dots \dots \dots (3)$$

where b' is the width (depth, that is, distance between surface and the grain boundary opposite to it) of the surface grain shown in Fig. 2. Eq. (3) is defined such that $R' = 1$ for the mean width ($b' = b/2$).

The boundary conditions for calculation are set as follows. The sides OA and OB are fixed in x - and z -directions, respectively, while unit tensile displacement is given on the side BC in x -direction. The side AC is kept free for the surface grains shown in Fig. 1(b),

Fig. 1 Models of polycrystals

Fig. 2 Area of calculation for grains near free surface

(*)1 Equation (1) may not be "anisotropy" in the strict meaning, as it only expresses the difference in elastic constant in one direction. However, as the present analysis assumes uniaxial loading and as the main objective is to present a proper model for the anisotropy of crystal, ϕ is called a parameter of anisotropy in the text. It is also assumed here that Young's modulus in the transverse direction is equal to that in the axial direction.

Fig. 3 Distributions of constraint ratios in grains near free surface and interior grains ($R = R' = 1$)

while the displacement $-v_0 R$ in z -direction is given for the interior grain shown in Fig. 1(a)⁽¹⁾.

Strain ϵ_z and Young's modulus E of an arbitrary grain are represented as $\epsilon_z = \bar{\epsilon}_z + \Delta\epsilon_z$ and $E = \bar{E}_z + \Delta E_z$, where $\bar{\epsilon}_z$ is the mean strain for polycrystals. (The upper wavy line $\sim$ represents the mean value for polycrystals.) Constraint ratio η_z in the stress direction is defined by⁽⁴⁾

$$\eta_z = \frac{\Delta\epsilon_z}{(\Delta\epsilon_z)_\sigma} = \frac{-\bar{E}_z \Delta\epsilon_z}{\Delta E_z \bar{\epsilon}_z} \quad (4)$$

, where the suffixes σ and ϵ represent the values under constant stress condition and constant strain condition, respectively. Also, $\eta_z = 1$ and $\eta_z = 0$ correspond to the deformation under constant stress and constant strain, respectively.

In the following calculations, Poisson's ratio and the parameter of anisotropy are taken as $\nu_0 = 0.3$ and $\psi = 0.8$, respectively, unless otherwise stated. Triangular elements are used in the finite element analysis where the number of elements is 200 for the region OACB⁽³⁾ (c.f. Fig. 12).

Fig. 4 Distributions of constraint ratios in grains near free surface and interior grains ($x/a = 1/20$, $R' = 1$)

Fig. 5 Distribution of constraint ratios in grains near free surface ($R = 1$)

2. 2. Results

2. 2. 1. Distribution of η_z

Fig. 3 shows the distribution of constraint ratios η_z in the stress direction for $R = R' = 1$. The solid and the broken lines show the distributions of η_z in the grains near the free surface and in the interior grains, respectively (The term "grains near free surface" means the surface grains and the inner grains adjacent to them (Fig. 2)). There is a difference between the distributions in both grains, especially in the very thin surface layer in the surface grain (approximately a quarter of the grain depth b' from the surface) as is shown by A in the figure. The difference, however, is very small. This implies that the difference in the distributions of stresses σ_z and strains ϵ_z in both grains is also very small (it is also shown in Fig. 3 that the difference between the values of constraint ratio in the surface grains calculated under plane stress ($\sigma_y = 0$) and plane strain ($\epsilon_y = 0$) is small, just as in the case of the interior grains⁽¹⁾⁽²⁾).

The mean values $\bar{\eta}_z$ of constraint ratio for the surface grains (the mean value for the region DACF in Fig. 2) and the inner grains (the region ODFB in Fig. 2) are 0.767 and 0.791, respectively, for the case of $R = R' = 1$ under plane stress condition ($\sigma_y = 0$). Meanwhile, the mean value for the interior grains (the region OACB in Fig. 1(a)) is 0.756, and the differences are relatively small. (The mean values for the surface grains and the inner grains under plane strain ($\epsilon_y = 0$) are 0.771 and 0.798, respectively.)

Fig. 4 shows the distribution of η_z for different values of R . It is also seen that the difference between the solid and the broken lines is small in both cases, especially for a large value of R such as $R = 2$ shown in Fig. 4(a).

Fig. 5 shows the distribution of constraint ratios η_z for different values of R' plotted against z/b where R is kept constant at $R = 1$. The broken line is a cosine curve given by Eq. (7) ($x/a = 0$) mentioned afterwards.

Fig. 6 Rotation of grains near free surface ($R = R' = 1$)

It is concluded from the above result of calculation that the distribution of η_z in the surface grain is scarcely affected by free surface except in a very thin surface layer and the shape of distribution is approximately represented with a cosine curve, just as in the case of the interior grain⁽²⁾.

Fig. 6 shows the motion of several points in the area OACB shown in Figs. 1(a) and (b) after deformation, where the sides OA and OB are fixed. The value indicated in the figure is the relative displacement of each point in the surface grains, where the side AC is free. Meanwhile, the values in the parentheses are those for the interior grains. It is seen that the grains rotate in the direction M shown in the figure when AC is free. It seems that the larger value of η_z in the inner grain than in the interior grain shown with B in Fig. 3 results from the rotation of grains near the surface. Although the rotation of grains disappears in elastic deformation after unloading, similar geometrical rotation of a certain group of grains near the free surface is likely to cause surface roughening of polycrystals after plastic deformation. There are fourfold points of grain boundary in the model of poly-

crystals used in the present analysis as shown with G in Fig. 1(a) and (b). It is expected that greater rotation appears in such a case of fourfold points, for the rotation of group of grains may be affected by the configuration of grains. Further discussion on this point, however, will be made in future.

2. 2. 2. Distributions of σ_z , ϵ_z and η_z

Although η_z mentioned above is hardly affected by the condition of free surface except in a very thin surface layer, it is a problem how deep the condition of constant stress reaches from the specimen surface (the constant stress condition is written as $\sigma_z = 0$ at free surface, and also as $\eta_z = 1$ from Eq. (5) defined later). To find out about this point, the distributions of stresses σ_z , strains ϵ_z and constraint ratios η_z in the normal direction to specimen surface are calculated.

Figs. 7 and 8 show distributions of σ_z and ϵ_z in the grains near specimen surface (solid lines), as well as that in the interior grains (broken lines). ϵ_0 is the mean strain in the stress direction (x-direction). The value of σ_z in the surface grain is about 1/4-

Fig. 7 Distributions of stresses and strains normal to free surface in grains near surface and interior grains ($R = R' = 1$, $x/a = 1/20$)

Fig. 9 Distributions of constraint ratios normal to free surface in grains near surface and interior grains ($R = R' = 1$)

Fig. 8 Distributions of stresses and strains normal to free surface in grains near surface and interior grains ($R = R' = 1$, $x/a = 19/20$)

Fig. 10 Distribution of constraint ratios η_z normal to surface grain and inner grain for various values of R' ($R = 1$)

Axi-symmetric triangular elements shown in Fig. 12 are used in finite element analysis⁽⁷⁾. The number of elements is 200. The unit displacement in the direction of stress axis and the displacement $-\nu_0 R/\sqrt{2}$ perpendicular to the stress axis on the side AC are given as boundary conditions.

3. 2. Results

The bold lines (the solid and the broken lines) in Fig. 13 show the distribution of constraint ratios η_x in the stress direction in the cylindrical grains. The value of η_x is large in the central region of the grain, while it reduces to almost zero at the grain boundary (DF in Fig. 12). The results for a plane model of grains⁽²⁾ are shown for the sake of comparison with the fine solid and the fine broken lines. The value of η_x for a cylindrical model of grains is lower than that for a plane model of grains, which results from strong three-dimensional restriction of grains.

Fig. 14 shows the relation between η_x and the aspect ratio R , where η_x is the mean value of constraint ratio for the inner grains averaged over the cylindrical region ODFB in Fig. 12 (volume average). Figs. 14(a) and (b) show the effects of parameter ϕ of anisotropy and Poisson's ratio ν_0 , respectively. The broken line shows the result for a plane model of grains⁽²⁾. The changes of η_x with R for the cylindrical and the plane models are similar, though the absolute values are different.

4. Discussion

The mean value of constraint ratio for polycrystals is linearly related to Young's modulus of polycrystals⁽⁴⁾. As the distribution of constraint ratios η_x near $x/a=0$ in the interior grain is well approximated with a cosine curve in many cases⁽²⁾ (c.f. Figs. 5 and 15), the following discussions are made on the relation among distribution of η_x , and its mean value and the effect of free surface on the mean value, by approximating

the distribution with a simple function based on the cosine curve.

4. 1. Plane and axi-symmetric models of interior grains

The distributions of η_x calculated by finite element method for various positions of x/a of the plane model of the interior grains (Fig. 1(a)) are shown in Fig. 15, where the broken line is a cosine curve given by $\eta_x = \left| \cos \frac{\pi x}{a} \right|$

Fig. 16(a) and (b) show the distributions of η_x in the cases of $R=1/2$ and $1/4$, respectively. (The horizontal length of the figure has been multiplied by R .) Considering these distributions shown in Figs. 15 and 16 together with the result⁽⁴⁾ that $\eta_x=1$ at the grain boundary perpendicular to the stress axis ($x/a=1/2$), the distribution of η_x in grains may be approximated by the following function.

Fig. 14 Relation between η_x and R for cylindrical model of grain

Fig. 13 Distribution of constraint ratios in stress (axial) direction in cylindrical grain

$$\left. \begin{aligned} \eta_z(z, x, R) &= \left| \cos \frac{\pi z}{a} \right|^m \quad (0 \leq z/a \leq 1) \\ m &= 1 \quad [0 \leq x/a \leq (1-R)/2] \quad (R < 1) \\ m &= (1-2x/a)/R \quad [(1-R)/2 < x/a \leq 1/2] \quad (R < 1) \\ m &= 1-2x/a \quad (R \geq 1) \\ \eta_z(z, x, R) &= \eta_z(0, x, R) = 1 \quad (z/a < 0, \\ &\quad \text{or } z/a > 1) \end{aligned} \right\} \dots\dots\dots(7)$$

The denominator in cosine in Eq. (7) is taken as a , because only the cross point of the ordinate and the cosine curve changes with R as shown in Figs. 15 and 16⁽²⁾. Examples of distribution of η_z given by Eq. (7) are shown in Fig. 17 for the range $z/b \leq 1/2$, which corresponds to the calculated result by finite element method as shown in Fig. 15.

The mean constraint ratio $\bar{\eta}_z(R)$ for polycrystals composed of grains with aspect ratio R can be calculated from Eq. (7) as follows.

$$\bar{\eta}_z(R) = \frac{4}{Ra^2} \int_0^{a/2} \int_{a(1-R)/2}^{a/2} \eta_z(z, x, R) dz dx \dots\dots\dots(8)$$

In the case of $R=1$, we have

$$\bar{\eta}_z(1) = 0.78 \dots\dots\dots(9)$$

Fig. 15 Distributions of constraint ratios in stress direction for several positions of x of interior grains ($R = 1$, $\phi = 0.8$)

Fig. 17 Assumed distribution of constraint ratios

, which is close to the value $\bar{\eta}_z = 0.76$ calculated with a plane model of polycrystals shown in Fig. 1(a) ($\phi = 0.8$, plane stress). Therefore, the approximation of η_z in Eq. (7) is considered appropriate for the plane model of the interior grain.

Fig. 18 shows the distribution of η_z in cylindrical (inner) grain for various values of R , where the grain boundary is set at the same position on the abscissa. Although the distribution is similar to that in the case of a plane model, the absolute value of η_z is lower than the cosine curve (broken line) mentioned above, especially in the central region of grains, owing to the three-dimensional restriction from the neighbor grains.

η_z becomes, however, close to 1 for larger values of R than 1. So, we assume the shape of distribution of η_z shown in Fig. 18, by the modification of Eq. (7) as follows.

Fig. 16 Distributions of constraint ratios in stress direction for several positions of x of interior grains ($\phi = 0.8$)

Fig. 18 Distribution of constraint ratios in stress direction in cylindrical grain

$$\left. \begin{aligned} \eta_s(r, x, R) &= \left[\cos \left\{ C \frac{\pi(r+ch)}{h} \right\} \right]^m \\ &\quad \left(-c \leq \frac{r}{h} \leq \frac{1}{2} \right) \\ m=1 \quad [0 \leq x/h \leq (1-R/2)/2] \quad (R < 2) \\ m=2(1-2x/h)R \quad [(1-R/2)/2 \\ &\quad < x/h \leq 1/2] \quad (R < 2) \\ m=1-2x/h \quad (R \geq 2) \\ \eta_s(r, x, R) &= \eta_s(-ch, x, R) = 1 \quad (r/h < -c) \end{aligned} \right\} \dots\dots\dots(10)$$

, where C ($C \leq 1$) and c are constants. In the expression of the exponent m , R in Eq. (7) is replaced by $R/2$ in Eq. (10), because the restriction in three-dimensional case is nearly twice stronger than that in two-dimensional case as discussed later (c.f. Fig. 19), and so in the former case the distribution of η_s changes quickly in the x -direction from the boundary perpendicular to x -axis.

As $\eta_s = 0$ at the grain boundary $r = Rh/2$, there is a relation between the constants C and c .

$$c = (1-C)/(2C) \dots\dots\dots(11)$$

The value of constraint ratio at $r = x = 0$ for $R = 1$ is given from Eqs. (10) and (11) as follows.

$$\eta_s(0, 0, 1) = \cos \left\{ \frac{\pi}{2} (1-C) \right\} \dots\dots\dots(12)$$

The mean constraint ratio $\bar{\eta}_s(R)$ for polycrystals is given for the cylindrical grain from Eq. (10) as follows, similarly to Eq. (9).

$$\begin{aligned} \bar{\eta}_s(R) &= \frac{16}{R^2 h^3} \\ &\times \int_0^{h/2} \int_0^{Rh/2} r \eta_s \left\{ r + (1-R) \frac{h}{2}, x, R \right\} dr dx \end{aligned} \dots\dots\dots(13)$$

If C is assumed to be 1 in Eq. (10), we have $\bar{\eta}_s(1) = 0.66$ for $R = 1$ from Eq. (13). On the other hand, the mean constraint ratio $\bar{\eta}_s$ for $R = 1$ calculated by finite element method with the cylindrical grains shown in Fig. 1(c) is $\bar{\eta}_s = 0.52$. Therefore, C is determined such that the calculated mean constraint ratio from Eqs. (10), (11) and (13) coincides with the calculated value by finite element method. Thus, we have

$$C = 0.858 \quad [\bar{\eta}_s(1) = 0.52] \dots\dots\dots(14)$$

The distribution of η_s obtained from Eqs. (10), (11) and (14) for $x/a = 0$ is shown with a dotted line in Fig. 18.

Fig. 19 Cross section and grain boundary of respective models of interior grains seen from stress direction

4. 2. Cubic model of interior grains

A grain is surrounded and restricted in two directions z and y in the case of cubic grains. It is not easy to calculate stress and strain distributions in three-dimensional cubic grains using finite element method, because the capacity of the memory of computer and the time required for the calculation might become too large when sufficient accuracy is needed. The distribution of constraint ratios η_s in cubic grain, however, can be estimated as follows based on the result on axi-symmetric three-dimensional model of grains shown in Eq. (10).

$$\left. \begin{aligned} \eta_s(z, y, x, R_z, R_y) &= f(z, x) f(y, x) \\ f(z, x) &= \left[\cos \left\{ C \frac{\pi(z+ca)}{a} \right\} \right]^m \\ f(y, x) &= \left[\cos \left\{ C \frac{\pi(y+ca)}{a} \right\} \right]^n \\ &\quad (-c \leq z/a, y/a \leq 1/2) \\ m=1 \quad [0 \leq x/a \leq (1-R_z/2)/2] \quad (R_z < 2) \\ m=2(1-2x/a)/R_z \quad [(1-R_z/2)/2 \\ &\quad < x/a \leq 1/2] \quad (R_z < 2) \\ m=1-2x/a \quad (R_z \geq 2) \\ n=1 \quad [0 \leq x/a \leq (1-R_y/2)/2] \quad (R_y < 2) \\ n=2(1-2x/a)/R_y \quad [(1-R_y/2)/2 \\ &\quad < x/a \leq 1/2] \quad (R_y < 2) \\ n=1-2x/a \quad (R_y \geq 2) \\ f(z, x) &= 1 \quad (z/a < -c) \\ f(y, x) &= 1 \quad (y/a < -c) \end{aligned} \right\} \dots\dots\dots(15)$$

, where R_z and R_y are the aspect ratios in z - and y -direction, respectively ($R_z = b_z/a$, $R_y = b_y/a$).

It is considered that the ratio of the area of grain boundary parallel to stress axis to the cross sectional area of the grain perpendicular to the stress axis is important for mutual restriction of grains. The situation is shown schematically in Fig. 19, where the cross sectional area perpendicular to the stress axis is shown for respective models of grains. The bold line shows a grain boundary parallel to the stress axis, while the fine line shows free surface. The ratio of the grain boundary area to the cross sectional area is denoted by ξ , where the length of grain in the stress direction is taken as unity. Let us consider the mean constraint ratio $\bar{\eta}_s$ for the cases of having the same ξ . The values of $\bar{\eta}_s$ for the cylindrical grain of $R = 1$ and the plane rectangular grain of $R = 1/2$, for example, are 0.52 and 0.49, respectively and very close to each other, where $\xi = 4$ in both cases (Fig. 14(a)). Thus, it may be said that the distribution curve of η_s is strongly dependent on the ratio ξ of grain boundary area.

The ratio ξ for the cylindrical grain is equal to that of the cubic grain for the same value of R . So, it is assumed that the shape of distribution curve of η_s , namely the constant C in Eq. (15) for the cubic grain is the same as that for the cylindrical grain (Eq. (14)).

The mean value $\bar{\eta}(R)$ of constraint

ratio for the cubic grain is calculated from Eq. (15) as follows.

$$\bar{\eta}_s(R_s, R_y) = \frac{8}{R_s R_y a^3} \int_0^{a/2} \int_{a(1-R_y)/2}^{a/2} \int_{a(1-R_s)/2}^{a/2} \eta_s(z, y, x, R_s, R_y) dz dy dx \quad (16)$$

For $R_s = R_y = 1$, substituting Eq. (15) and $C = 0.858$ into Eq. (16), we have

$$\bar{\eta}_s(1, 1) = 0.45 \quad (17)$$

The relations between $\bar{\eta}_s(R)$ or $\bar{\eta}_s(R, R)$ and R for plane, cylindrical and cubic models of grains calculated from Eqs. (8), (13) and (16) are shown with dotted lines ①, ② and ③, respectively.

4. 3. Plane and cubic models of surface grains

The calculated distribution of η_s in the surface grain is also approximated with a cosine curve as is shown with the broken line in Fig. 5. So, it is considered that Eqs. (7) and (15) for a plane model and a cubic model, respectively, are valid for the surface grains and similar discussion as above is applicable to the surface grains. The case of $R=1$ is considered representatively in the following.

When the surface of metal polycrystals is finished with machines, it is expected that the surface cuts grains randomly and hence the width (depth) of surface grains distributes randomly. Then, it is possible to estimate the mean value $\bar{\eta}_{ss}$ of constraint ratio in the surface grains by taking the average of distributions of η_s for various widths or R' . It may be reasonable to assume that the value of b' distributes uniformly in the range $0 \leq b' \leq b$ ($0 \leq R' \leq 2$), for the maximum value of the width b' of the surface grain is $b' = b$ ($R' = 2$). Thus, the mean value $\bar{\eta}_{ss}(R)$ of constraint ratio for surface grain is obtained by integrating for various positions R' of the surface ($0 \leq R' \leq 2$).

In the case of a plane model of grains, we have from Eq. (8)

$$\bar{\eta}_{ss}(R) = \frac{2}{Ra^2} \int_0^2 \frac{1}{R'} \times \int_0^{a/2} \int_{a(1-RR')/2}^{a/2} \eta_s(z, x, R') dz dx dR' \quad (18)$$

For $R=1$, substituting Eq. (7) into Eq. (18), we have after numerical integration

$$\bar{\eta}_{ss}(1) = 0.59 \quad (19)$$

Similarly, the mean value of constraint ratio for polycrystals of cubic grains is given considering the case of $R_s = R_y = R$ in Eq. (16).

$$\bar{\eta}_{ss}(R) = \frac{4}{R^2 a^3} \int_0^2 \frac{1}{R'} \int_0^{a/2} \int_{a(1-RR')/2}^{a/2} \int_{a(1-R)/2}^{a/2} \eta_s(z, y, x, R', R) dy dz dx dR' \quad (20)$$

For $R=1$, substituting Eq. (15) into Eq. (20), we have

$$\bar{\eta}_{ss}(1) = 0.40 \quad (21)$$

The ratio of the mean value of constraint ratio of the surface grain to that of the interior grain of specimen for

$R=1$ is given from Eqs. (9), (17), (19) and (21) as follows.

$$\left. \begin{aligned} \bar{\eta}_{ss}(1)/\bar{\eta}_s(1) &= 0.75 \text{ for plane model of grains} \\ \bar{\eta}_{ss}(1)/\bar{\eta}_s(1) &= 0.89 \text{ for cubic model of grains} \end{aligned} \right\} \quad (22)$$

It is concluded that the mean value of constraint ratio for the surface grains decreases to 75 - 89 % of the mean value for the interior grain. Calculated values of the ratio $\bar{\eta}_{ss}(R)/\bar{\eta}_s(R)$ for different values of R from $R = 0.1$ to 4 show similar result. It is known⁽⁵⁾ that the experimental value of mean constraint ratio of surface grains is $\bar{\eta}_{ss} = 0.45 - 0.50$ which is calculated from X-ray elastic constant of α -iron, while the mean constraint ratio averaged over all polycrystals obtained from the experimental value of mechanical elastic constant is $\bar{\eta}_s = 0.67$ for α -iron. Thus, the experimental value of the ratio is $\bar{\eta}_{ss}/\bar{\eta}_s = 0.67 - 0.75$, which is consistent with the trend of the above analytical result (Eq. (22)).

It is known⁽⁴⁾⁽⁵⁾ that Young's modulus of polycrystals is approximately linearly dependent on the mean constraint ratio. Therefore, it is expected that the value of Young's modulus $\bar{E}$ of the surface grains is different from that of the interior grains if the mean value $\bar{\eta}_{ss}$ of constraint ratio for the surface grains differs from the mean value $\bar{\eta}_s$ of the interior grains. Although it was suggested⁽⁵⁾ that Young's modulus of surface layer decreases with an increase in η_s due to free surface, the effect seems to be restricted to a very thin layer in the surface grains as indicated with A in Fig. 3. On the contrary, the mean value of constraint ratio for surface grains decreases as shown in Eq. (22), which is expected to cause a larger value of $\bar{E}$ in the surface grains as is also shown from the experimental data of X-ray elastic constant (calculation considering the volume of grains, however, is necessary for more quantitative analysis).

The expression for distribution of constraint ratios in a simple function may be useful in future study on more complicated deformation behavior of polycrystals, though discussions are made only on the effect of surface of polycrystals in the present paper.

5. Conclusions

Deformation of polycrystalline metals under uniaxial loading is studied by analysing models of polycrystals by finite element method. Discussions are also made on the values of mean constraint ratio η_s in surface grain and interior grain, by representing the distribution of constraint ratios η_s in the stress direction with a simple cosine function. The results may be summarized as follows.

(1) The effect of free surface on distribution of constraint ratios η_s in stress direction is small and confined to a very thin layer near the surface. The distribution of η_s in the surface grains is approximately represented with a cosine

curve, similarly to that in the interior grains.

(2) The stress σ_s normal to surface is nearly equal to zero in the surface grain, while the strain ϵ_s or constraint ratio η_s normal to surface changes in the surface grain. The distribution of η_s is approximately represented with a cosine curve, that is, η_s is nearly equal to 1 at the surface, while it reduces to 0 at the grain boundary opposite to the surface.

(3) There is little effect of free surface on the distributions of stresses, strains and constraint ratios in the inner grains adjacent to the surface grains.

(4) Group of grains placed near surface is found to rotate during deformation.

(5) Although the distribution of η_s in the surface grain is approximately represented with a cosine curve similarly to that in the interior grain, the mean value $\bar{\eta}_{ss}$ of constraint ratio in the surface grain is different from the mean value $\bar{\eta}_s$ in the interior grain, that is, $\bar{\eta}_{ss}$ is about 75 - 89 % of $\bar{\eta}_s$, because the surface cuts grains randomly and hence the width (depth) of the surface grains distributes randomly from 0 to b , where b is the width of the interior grains.

(6) Three-dimensional restriction of grains in polycrystals is studied with a

cylindrical model of grains and the result is compared with that of a two-dimensional plane rectangular model of grains. Three-dimensional restriction is nearly double the two-dimensional one, for the strength of restriction of grain is nearly proportional to the area of grain boundary parallel to the stress axis and the area of boundary in three-dimensional grains is twice as wide as that in two-dimensional ones.

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