X-Ray Stress Measurement of Hexagonal Polycrystals with [001] Fiber Texture*

Keisuke TANAKA** and Yoshiaki AKINIWA**

A new method of X-ray measurements of tri-axial residual stresses was proposed for hexagonal polycrystals with the [001] fiber texture. The relation between X-ray strain and $\sin^2 \psi$ is linear for the cases of the fiber axis perpendicular or parallel to the specimen surface, provided that there is no shear stress acting on the specimen surface. The in-plane stresses, σ_{11} , σ_{22} , and σ_{12} , and the normal stress perpendicular to the specimen surface, σ_{33} , can be determined from the slope and the intercept of the linear regression line for the relation between X-ray strain and $\sin^2 \psi$ obtained for three different directions.

Key Words: X-Ray Stress Measurement, Residual Stress, Hexagonal Polycrystals, Fiber Texture

1. Introduction

X-ray stress measurements of polycrystals have been conducted with the $\sin^2 \psi$ method, where ψ is the angle between the normals of the diffraction plane and of the specimen surface. The stress value is determined from the slope of the linear regression line in the diagram of the strain measured by X-ray diffraction plotted against $\sin^2 \psi$. The relation between the strain and $\sin^2 \psi$ is not necessarily linear, when polycrystals have a preferred orientation or texture.

Hanabusa et al.⁽²⁾ have proposed a new method for X-ray stress measurement of aluminum nitride (AlN) thin films with the columnar structure having the [001] axis of hexagonal polycrystals perpendicular to the coating surface. They found that X-ray strain was a linear function of $\sin^2 \psi$ for the case of the equi-biaxial stress state. They further applied their method to measure equi-biaxial residual stresses in hexagonal zinc oxide (ZnO) films which have the [001] fiber texture perpendicular to the coating surface⁽³⁾. The fiber texture of hexagonal polycrystals has been observed for a variety of new materials. The

lamellar structures of titanium aluminide TiAl/Ti₃Al have the fiber texture of tetragonal TiAl [111] axis and hexagonal Ti₃Al [001] axis perpendicular to the lamellar plane^{(4),(5)}. In this case, the fiber direction is not necessarily perpendicular to the specimen surface. It can be parallel to the specimen surface.

In the present paper, a new method of X-ray measurements of non-equal biaxial and triaxial stresses was proposed for hexagonal polycrystals having the [001] fiber texture with the fiber axis perpendicular or parallel to the specimen surface.

2. Relation between X-ray Strain and Applied Stress

Specimen coordinates (P_i) are taken as shown in Fig. 1, where the P_3 axis is perpendicular to the specimen surface. Laboratory coordinates (L_i) have the orientation relation with P_i as shown in Fig. 1. The

Fig. 1 Coordinates of specimen system, P_i , laboratory system, L_i , and crystal system, X_i

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** Department of Mechanical Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan

Fig. 2 Transformation matrices of coordinates

crystalline coordinates (X_i) are also taken with the origin O. Transformation matrices among three coordinate systems are denoted by γ , π , ω as shown in Fig. 2. Stress and strain tensors are $(\sigma_{ij}, \epsilon_{ij})$, $(\sigma_{ij}^*, \epsilon_{ij}^*)$, and $(\sigma_{ij}^L, \epsilon_{ij}^L)$ for P_i , X_i , and L_i coordinates, respectively.

In the X-ray measurement, the normal strain ϵ_{33}^L along L_3 direction is measured. The relation of ϵ_{33}^L with the applied stress σ_{pq} is derived as follows.

Transformations of stress and strain are given as

$$\epsilon_{33}^L = \gamma_{3i} \gamma_{3j} \epsilon_{ij}^* \quad (1)$$

$$\sigma_{kl}^* = \pi_{pk} \pi_{ql} \sigma_{pq} \quad (2)$$

where repeated roman letters mean the summation convention from 1 to 3. Here, the macrostress σ_{pq} is assumed to act on each grain as in Reuss' model⁽⁶⁾. The stress-strain relation for single crystals is

$$\epsilon_{ij}^* = S_{ijkl} \sigma_{kl}^* \quad (3)$$

where S_{ijkl} is the elastic compliance. From Eqs. (1)–(3), we have

$$\epsilon_{33}^L = \gamma_{3i} \gamma_{3j} S_{ijkl} \pi_{pk} \pi_{ql} \sigma_{pq} \quad (4)$$

The elastic compliance S_{ijkl} of hexagonal crystals is expressed in the matrix notation as follows⁽⁷⁾:

$$\{S_{ij}\} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{13} & 0 & 0 & 0 \\ S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(S_{11} - S_{12}) \end{bmatrix} \quad (5)$$

The independent constants are S_{11} , S_{12} , S_{13} , S_{33} , and S_{44} . It should be noted that the above form of the matrix ensures transverse isotropy on the plane perpendicular to the [001] direction. Equation (4) can be rewritten as

$$\begin{aligned} \epsilon_{33}^L = & \gamma_{31}^2 (S_{11} \pi_{p1} \pi_{q1} + S_{12} \pi_{p2} \pi_{q2} + S_{13} \pi_{p3} \pi_{q3}) \sigma_{pq} \\ & + \gamma_{32}^2 (S_{12} \pi_{p1} \pi_{q1} + S_{11} \pi_{p2} \pi_{q2} + S_{13} \pi_{p3} \pi_{q3}) \sigma_{pq} \\ & + \gamma_{33}^2 \{ (S_{33} - S_{13}) \pi_{p3} \pi_{q3} \sigma_{pq} + S_{13} (\sigma_{11} + \sigma_{22} + \sigma_{33}) \} \\ & + \gamma_{32} \gamma_{33} S_{44} \pi_{p2} \pi_{q3} \sigma_{pq} + \gamma_{33} \gamma_{31} S_{44} \pi_{p3} \pi_{q1} \sigma_{pq} \\ & + 2 \gamma_{31} \gamma_{32} (S_{11} - S_{12}) \pi_{p1} \pi_{q2} \sigma_{pq} \end{aligned} \quad (6)$$

The transformation matrix ω is given by

$$\omega = \begin{bmatrix} \cos \phi \cos \phi & \cos \phi \sin \phi & -\sin \phi \\ -\sin \phi & \cos \phi & 0 \\ \sin \phi \cos \phi & \sin \phi \sin \phi & \cos \phi \end{bmatrix} \quad (7)$$

The matrix γ is related to ω and π as

$$\gamma_{ij} = \omega_{im} \pi_{mj} \quad (8)$$

3. [001] Fiber Axis Perpendicular to Specimen Surface

Let the [001] fiber axis coincides with the normal of the specimen surface P_3 shown in Fig. 1. By denoting the angle between $X_1[100]$ axis and P_2 axis as β , the transformation matrix π is given by

$$\pi = \begin{bmatrix} \cos \beta & \sin \beta & 0 \\ -\sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (9)$$

By substituting Eqs. (7) and (9) into (8), we have

$$\gamma = \begin{bmatrix} \cos \phi \cos (\phi + \beta) & \cos \phi \sin (\phi + \beta) & -\sin \phi \\ -\sin (\phi + \beta) & \cos (\phi + \beta) & 0 \\ \sin \phi \cos (\phi + \beta) & \sin \phi \sin (\phi + \beta) & \cos \phi \end{bmatrix} \quad (10)$$

The substitution of Eqs. (7), (9), and (10) into Eq. (6) leads to

$$\begin{aligned} \epsilon_{33}^L = & \{ S_{11} (\sigma_{11} \cos^2 \phi + \sigma_{22} \sin^2 \phi + 2 \sigma_{12} \cos \phi \sin \phi) \\ & + S_{12} (\sigma_{11} \sin^2 \phi + \sigma_{22} \cos^2 \phi - 2 \sigma_{12} \cos \phi \sin \phi) \\ & - (S_{33} - 2 S_{13}) \sigma_{33} - S_{13} (\sigma_{11} + \sigma_{22} + \sigma_{33}) \} \sin^2 \phi \\ & + S_{44} (\sigma_{23} \sin \phi + \sigma_{31} \cos \phi) \sin \phi \cos \phi \\ & + (S_{33} - S_{13}) \sigma_{33} + S_{13} (\sigma_{11} + \sigma_{22} + \sigma_{33}) \end{aligned} \quad (11)$$

It should be noted that the ϵ_{33}^L is independent of the crystal orientation angle β . This is because of transverse isotropy of hexagonal crystals. Since the elastic deformation of each grain does not cause any strain incompatibility, the stress in each grain is equal to the applied macrostress as assumed in Reuss' model.

When σ_{13} or σ_{32} is not zero, the measured strain is dependent not only on $\sin^2 \phi$, but also on $\sin 2\phi$. The strain measured at positive and negative ϕ will be different. For the cases of ϕ splitting, the stress can be determined by following the procedure similar to the one proposed by Dölle⁽⁸⁾ for randomly oriented polycrystals.

For the cases of $\sigma_{13} = \sigma_{32} = 0$, the relation between ϵ_{33}^L and $\sin^2 \phi$ is linear. For $\phi = 0^\circ$, we have

$$\epsilon_{33}^L = \{ (S_{11} - S_{13}) \sigma_{11} + (S_{12} - S_{13}) \sigma_{22} + (S_{13} - S_{33}) \sigma_{33} \} \sin^2 \phi + S_{13} (\sigma_{11} + \sigma_{22}) + S_{33} \sigma_{33} \quad (12)$$

For $\phi = 90^\circ$,

$$\epsilon_{33}^L = \{ (S_{12} - S_{13}) \sigma_{11} + (S_{11} - S_{13}) \sigma_{22} + (S_{13} - S_{33}) \sigma_{33} \} \sin^2 \phi + S_{13} (\sigma_{11} + \sigma_{22}) + S_{33} \sigma_{33} \quad (13)$$

and for $\phi = 45^\circ$,

$$\epsilon_{33}^L = \left\{ \frac{1}{2} (S_{11} + S_{12} - 2 S_{13}) (\sigma_{11} + \sigma_{22}) + (S_{13} - S_{33}) \sigma_{33} + (S_{11} - S_{12}) \sigma_{12} \right\} \sin^2 \phi + S_{13} (\sigma_{11} + \sigma_{22}) + S_{33} \sigma_{33} \quad (14)$$

Four stress components, σ_{11} , σ_{22} , σ_{33} and σ_{12} , can be obtained from the slope and the intercept of the linear regression lines of the relation between ϵ_{33}^L and $\sin^2 \phi$ for $\phi = 0^\circ$, 45° , and 90° .

When $\sigma_{33} = 0$ and $\sigma_{11} = \sigma_{22} = \sigma$, Eq. (12) or (13) is rewritten as

$$\varepsilon_{33}^L = (S_{11} + S_{12} - 2S_{13})\sigma \sin^2 \psi + 2S_{13}\sigma \quad (15)$$

The above equation was derived by Hanabusa et al.⁽²⁾ When the stress state is equi-biaxial, Eq. (15) is useful for stress measurement. For non-equi biaxial or triaxial cases, Eqs. (12) to (14) need to be used for stress measurement.

4. [001] Fiber Axis Parallel to Specimen Surface

The [001] fiber axis is now assumed to coincide with P_1 direction shown in Fig. 1. Because of transverse isotropy of hexagonal crystals, we can take X_1 and X_2 axes are parallel to P_2 and P_3 directions without loss of generality. In this case, the matrix π is

$$\pi = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad (16)$$

From Eqs. (7), (8) and (16), γ is given by

$$\gamma = \begin{bmatrix} \cos \psi \sin \phi & -\sin \phi & \cos \psi \cos \phi \\ \cos \phi & 0 & -\sin \phi \\ \sin \psi \sin \phi & \cos \psi & \sin \psi \cos \phi \end{bmatrix} \quad (17)$$

By substituting Eqs. (16) and (17) into Eq. (6), we have

$$\begin{aligned} \varepsilon_{33}^L = & \{S_{11}(\sigma_{22} \sin^2 \phi - \sigma_{33}) + S_{13}(-\sigma_{11} + \sigma_{22} + \sigma_{33}) \\ & \times \cos^2 \phi + S_{33}\sigma_{11} + S_{44}\sigma_{12} \cos \phi \sin \phi\} \sin^2 \psi \\ & + \{S_{44}\sigma_{31} \cos \phi + 2(S_{11} - S_{12})\sigma_{23} \sin \phi\} \sin \psi \cos \psi \end{aligned} \quad (18)$$

When σ_{13} or σ_{32} is not zero, the measured strain is dependent not only on $\sin^2 \psi$, but also on $\sin 2\psi$. This ψ splitting can also be dealt with the method described above.

When $\sigma_{23} = \sigma_{31} = 0$, the relation between ε_{33}^L and $\sin^2 \psi$ is linear. For $\phi = 0^\circ$, we have

$$\varepsilon_{33}^L = \{(S_{33} - S_{13})\sigma_{11} + (S_{13} - S_{12})\sigma_{22} + (S_{13} - S_{11})\sigma_{33}\} \sin^2 \psi + S_{13}\sigma_{11} + S_{12}\sigma_{22} + S_{11}\sigma_{33} \quad (19)$$

For $\phi = 90^\circ$,

$$\varepsilon_{33}^L = \{(S_{11} - S_{12})\sigma_{22} + (S_{12} - S_{11})\sigma_{33}\} \sin^2 \psi + S_{13}\sigma_{11} + S_{12}\sigma_{22} + S_{11}\sigma_{33} \quad (20)$$

and for $\phi = 45^\circ$,

$$\varepsilon_{33}^L = \frac{1}{2} \{(2S_{33} - S_{13})\sigma_{11} + (S_{11} + S_{13})\sigma_{22} + (S_{13} - 2S_{11})\sigma_{33}$$

$$+ S_{44}\sigma_{12}\} \sin^2 \psi + S_{13}\sigma_{11} + S_{12}\sigma_{22} + S_{11}\sigma_{33} \quad (21)$$

As in the preceding section, four stress components, σ_{11} , σ_{22} , σ_{33} and σ_{12} can be obtained from the slope and the intercept of linear regression lines of the relation between ε_{33}^L and $\sin^2 \psi$ for $\phi = 0^\circ$, 45° , and 90° .

5. Conclusions

A new method of X-ray measurement of tri-axial residual stresses was proposed for hexagonal polycrystals with the [001] fiber texture. The relation between the strain measured by X-ray diffraction and $\sin^2 \psi$ is linear for the cases of the fiber axis perpendicular or parallel to the specimen surface, provided that there is no shear stress acting on the specimen surface. The in-plane stresses, σ_{11} , σ_{22} , and σ_{12} , and the normal stress perpendicular to the specimen surface, σ_{33} , are determined from the slope and the intercept of linear regression lines for the relation between X-ray strain and $\sin^2 \psi$ obtained for three different directions: $\phi = 0^\circ$, 45° , and 90° . This method is an extension of the conventional $\sin^2 \psi$ method for polycrystals with random orientation.

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