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General paper

Modeling and Simulation of X-Ray Stress Measurement Using PSPC as a Detector

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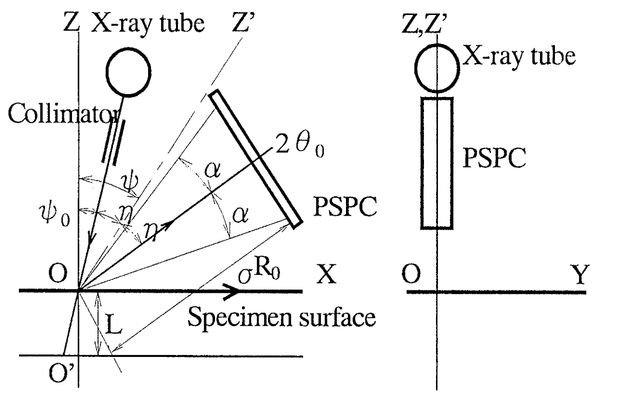
Abstract: Recently, the position sensitive proportional counter (PSPC) has been becoming popular as a detector for X-ray stress measurement. However, little information is available in the literature regarding the effects of specimen mis-setting and/or collimator misalignment on the stress measurement. Many factors such as the stress and the X-ray diffraction broadening of the specimen, the X-ray focus size, the dimensions of the collimator, the PSPC and the goniometer are complicatedly related to the effects of specimen mis-setting and/or collimator misalignment. In this paper, a modeling of the X-ray stress measurement using a PSPC as the detector is presented enabling us to simulate the stress measurement under various conditions. In the case of Ω assembly, the errors in stress measurement are illuminated under specimen mis-setting and/or collimator misalignment.

Keywords: *X-ray stress measurement, Position sensitive proportional counter, Collimator, Mis-setting and misalignment, Ω assembly*

1. INTRODUCTION

Recently, the position sensitive proportional counter (PSPC) has been becoming popular as a detector for X-ray stress measurement. However, little information is available in the literature regarding the effects of specimen mis-setting and/or collimator misalignment on stress measurement using a PSPC, though such information is a priority matter in X-ray stress measurement [1].

Many factors such as the stress and the X-ray diffraction broadening of a specimen, the X-ray focus size, the dimensions of the collimator, the PSPC and the goniometer are complicatedly related to the effects of specimen mis-setting and/or collimator misalignment.



(a) Z-O-X plane (b) Z,Z'-O-Y plane

Fig.1. Ω assembly X-ray stress analyzer using a collimator and PSPC.

This is why no one has successfully demonstrated the phenomena of specimen mis-setting and/or collimator misalignment. One of the authors started with the case of a Ψ assembly (the side inclination method) to study the effect of specimen mis-setting on the stress measurement using a PSPC as the detector [2]. Taking the factors mentioned above into account, a model of X-ray stress measurement was made in order to conduct a simulation of the measurement. It was found that the model is well applicable to estimate the errors in stress measurement for both specimen mis-setting and also for collimator misalignment.

In this paper, an X-ray stress measurement model using a PSPC as the detector is presented for the case of an Ω assembly (the iso-inclination method). And the errors in stress measurement are illuminated under specimen mis-setting and/or collimator misalignment.

2. MODEL OF X-RAY STRESS MEASUREMENT

2.1. X-ray Stress Analyzer

The stress analyzer used in this study is schematically illustrated in Fig. 1. The X-ray focus is wide enough to cover the entrance area of the collimator. The PSPC is fixed at a distance R_0 from the goniometer center O. An X-ray hits the specimen with zero stress from the direction of ψ_0 and is diffracted to position $2\theta_0$ on the PSPC. The angle α indicates the half-range of the diffraction angle detectable by the PSPC. L is the offset of the

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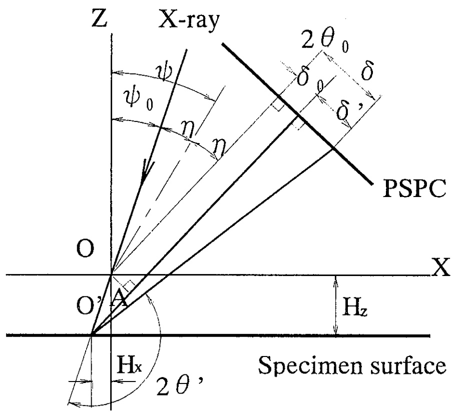

Fig. 2. Peak shift caused by specimen mis-setting.

mis-set specimen in the direction of the Z-axis, which is normal to the specimen surface.

2.2. Peak Shift Caused by Specimen Mis-setting

Figure 2 shows the peak shift δ_0 of the diffraction profile on the PSPC caused by the mis-setting of H_z, that is L. L is defined positive when the specimen is mis-set over the goniometer center O. If the specimen has a stress σ, the diffraction angle changes to $2\theta_0'$ from $2\theta_0$ and, therefore, the peak shift occurs further by δ'. δ_0 is expressed by

$$\delta_0 = L \cdot \sin 2\eta / (\cos\psi_0 \cdot \Delta\alpha). \quad (1)$$

$2\theta_0'$ is

$$2\theta_0' = (\sigma / K) \cdot \sin^2\psi + 2\theta_0$$
$$-\{\nu / K(1+\nu)\} \cdot (\sigma_1 + \sigma_2), \quad (2)$$

where K is the stress constant, ν is Poisson's ratio, σ_1 and σ_2 are principal stresses. δ' is

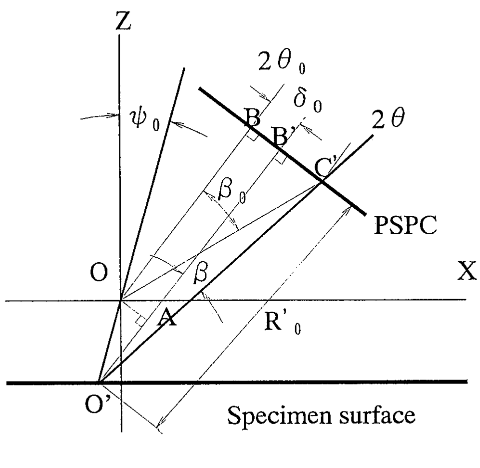

Fig. 3. X-ray path to PSPC.

$$\delta' = (R_0 - \Delta R) \cdot \tan(2\theta_0' - 2\theta_0) / \Delta\alpha, \quad (3)$$

where

$$\Delta\alpha = R_0 \cdot \tan\alpha / \alpha, \quad (4)$$

$$\Delta R = L \cdot \cos 2\eta / \cos\psi_0. \quad (5)$$

Then, the peak position of the X-ray on the PSPC is expressed by the diffraction angle $2\theta_1$, which is given as

$$2\theta_1 = 2\theta_0 + \delta_0 + \delta'. \quad (6)$$

2.3. X-ray Intensity Detected by the PSPC

As is shown in Fig. 3, the intensity $I_{\beta 0}$ of the X- ray, which comes from the point O' of the mis-set specimen and is detected by the PSPC at an arbitrary position C', can be expressed as

$$I_{\beta 0} = I_0 \cdot \Delta\alpha \cdot \cos\beta \cdot \{R_0 / (R_0' / \cos\beta)\}^2, \quad (7)$$

where I_0 is the unit intensity and β is given by the following equation;

$$\beta = R_0 \cdot (\beta_0 - \delta_0) / R_0', \quad (8)$$

where $\beta_0 = 2\theta - 2\theta_0$ and

$$R_0' = R_0 - \Delta R. \quad (9)$$

If the diffraction profile is assumed to be a Gaussian distribution against diffraction angle 2θ with its center at $2\theta_1$, the X-ray intensity $I_{2\theta}$ at 2θ of the PSPC diffracted from point O' of the specimen is given as

$$I_{2\theta} = I_0 \cdot \Delta\alpha \cdot \cos\beta \cdot (\cos\beta / R_0')^2$$
$$\cdot \exp\{-b^2(2\theta - 2\theta_1)^2\}, \quad (10)$$

where b is a parameter indicating the half-value breadth of the diffraction profile.

2.4. X-ray through the Collimator

Figure 4 shows a collimator settled in the side of the incident beam. Let us consider an X-ray UD. Position U is defined by the distance x'_ψ from the center of the incident beam at the entrance of the collimator. Position D is defined by the distance x_ψ from the center of the incident beam at the specimen surface O'. Point O" is the point hit by the X-ray. Then, the increase in the incident angle $\Delta\psi$ of the X-ray is expressed as

$$\Delta\psi = (x'_\psi - x_\psi) / (Cl + L / \cos\psi_0), \quad (11)$$

where Cl is the effective length of the collimator and is given as the distance from the entrance to the goniometer

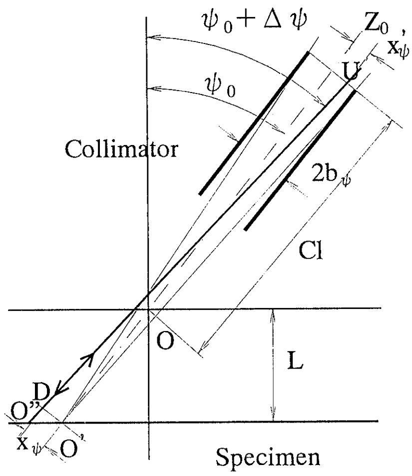

Fig. 4. X-ray path through collimator.

center O.

Figure 5 shows the path O"C" of the X-ray UD to PSPC. Make a line O"B" parallel to the line OB from point O" and let the line O'E be the normal line from point O' to the line O"B".

Let the distance between the points O' and O" be expressed by ζ and the angle $\angle$EO"O' by γ. Then, the peak shift δ_{0c} of the X-ray is given by the following equation for the case of zero stress.

$$\delta_{0c} = \{(L \cdot \sin 2\eta / \cos\psi_0 - \zeta \cdot \sin\gamma) - R_{0c}' \cdot \tan\Delta\psi\} / \Delta\alpha, \tag{12}$$

where R_{0c}' is given as

$$R_{0c}' = R_0 - \Delta R - \zeta \cdot \cos\gamma. \tag{13}$$

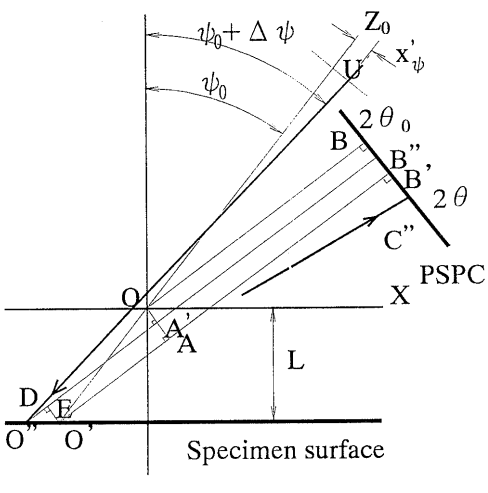

Fig. 5. X-ray path to PSPC.

The additional peak shift δ_c' is expressed as

$$\delta_c' = R_{0c}' \cdot \tan(2\theta_{0c}' - 2\theta_0) / \Delta\alpha, \tag{14}$$

where $2\theta_{0c}'$ is the diffraction angle of the X-ray UD for the stressed specimen and is given as

$$2\theta_{0c}' = (\sigma / K) \cdot \sin^2(\psi + \Delta\psi) + 2\theta_0 - \{\nu / K(1+\nu)\} \cdot (\sigma_1 + \sigma_2). \tag{15}$$

Finally the X-ray intensity $I_{2\theta}$ at 2θ of the PSPC diffracted from point O" of the specimen is given as

$$I_{2\theta} = I_0 \cdot \Delta\alpha \cdot \cos\beta_c' \cdot (\cos\beta_c' / R_{0c}')^2 \cdot \exp\{-b^2(2\theta - 2\theta_{1c})^2\}, \tag{16}$$

where β_c' and $2\theta_{1c}$ are

$$\beta_c' = R_0 \cdot (\beta_0 - \delta_{0c}) / R_{0c}', \tag{17}$$

$$2\theta_{1c} = 2\theta_0 + \delta_{0c} + \delta_c'. \tag{18}$$

ζ and γ are given as

$$\zeta = x_\psi \cdot \sin(\pi/2 + \Delta\psi) / \sin\{\pi/2 - (\psi_0 + \Delta\psi)\}, \tag{19}$$

and

$$\gamma = 2\theta_0 - \pi/2 - \psi_0. \tag{20}$$

2.5. X-ray Diffraction Profile

Equation (16) is applicable to calculate the diffraction intensity $I_{2\theta}$ for almost all of combinations of X- rays and specimens. Therefore, it is easily understood that the X-ray diffraction profile at incident angle ψ_0 is given by integrating $I_{2\theta}$ at x'_ψ and x_ψ from $-b_\psi$ to b_ψ for both x as shown in Fig. 6 (a).

If the collimator is settled with a misalignment of translation t or/and rotation κ, the diffraction profile is given by the integration method corresponding to each misalignment as shown in Figs. 6 (b)~(d).

3. SIMULATION OF X-RAY STRESS MEASUREMENT

3.1. Conditions for Simulation

The conditions used in simulation of X-ray stress measurement for specimen mis-setting and/or collimator misalignment are shown in Table 1. Steel is assumed to be measured using a chromium target by the Ω method with four incident angles of 0, 15, 30 and 45 deg. The determination of the peak displacement was done using

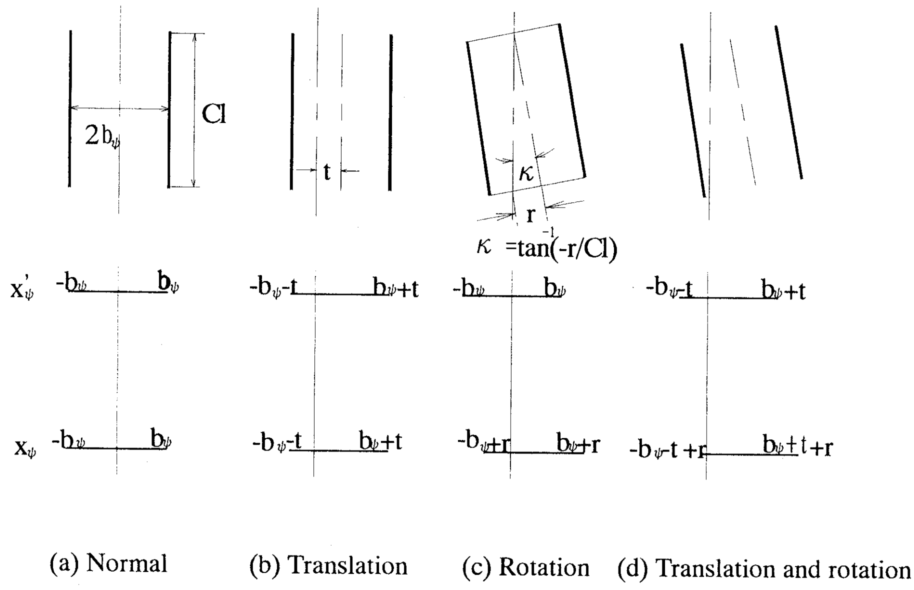

Fig. 6. Collimator misalignment and the integration method of diffraction intensity.

the mid-chord method [1]. The stress value was calculated from the slope M of $2\theta - \sin^2\psi$ diagram and the stress constant K using the following equation:

$$\sigma_x = M \cdot K. \tag{21}$$

3.2. Intrinsic Stress Caused by the Collimator

Even if we measure a specimen with zero stress under normal conditions, the slope of $2\theta - \sin^2\psi$ diagram is not zero, it is positive when we use a wider and/or shorter collimator. This is caused by the component of the incident beam having the additional incident angle $\Delta\psi$, which is shown in Fig. 4. Let us call the stress value corresponding to the slope the intrinsic stress σ_c. The intrinsic stress calculated for the goniometer radius R_0 = 200 mm and for the half-value breadth HVB = 2 deg are shown in Tables 2 (a) and (b), respectively. It is seen that the absolute value of σ_c increases with the increase in the width of the collimator and decreases with the increase in its effective length. The goniometer radius and half-value breadth of the specimen also change the value of σ_c. The effect of principal stresses on the intrinsic stress was found negligible.

3.3. Error in Stress Measurement due to Specimen Mis-setting

If we conduct stress measurement of mis-set specimen using the line incident beam, it was found [2] that the intrinsic stress is zero and the error $\Delta\sigma_x$ in the stress measurement can be expressed by a linear equation of the ratio L / R_0 as

$$\Delta\sigma_x = \sigma_x - \sigma = -4500 \cdot L / R_0. \tag{22}$$

Equation (22) is independent of the stress and the half-value breadth of the specimen, and it depends strongly on the conditions concerning the incident angles adopted in the measurement. When using a collimator, it is important to take the intrinsic stress σ_c into account for the discussion of the error. The ratio $2b_\psi/Cl$ effectively expresses the error. This is seen in Fig. 7, which shows that we can relate the difference in stress value σ_x at a given L/R_0 and at L/R_0 = 0 to $2b_\psi/Cl$ as one line. The stress value σ_x at L/R_0 = 0 is equal to $\sigma + \sigma_c$. Little influence of the half-value breadth and the stress of the specimen on the relationship is seen in the figure.

Let us, therefore, define the pure error $\Delta\sigma_L$ due to specimen mis-setting as

$$\Delta\sigma_L = \sigma_x - \sigma - \sigma_c. \tag{23}$$

Figure 8 is the plotting of $\Delta\sigma_L$ versus L/R_0. It is seen that the relationship between $\Delta\sigma_L$ and L/R_0 is linear, depends on $2b_\psi/Cl$ and is given by

$$\Delta\sigma_L = -4500 \cdot \{1 - 1.24\,(2b_\psi/Cl) - 4.28\,(2b_\psi/Cl)^2\} \times L/R_0 \quad \text{(MPa)}. \tag{24}$$

3.4. Error in Stress Measurement Due to Collimator Misalignment

Let us define the pure error due to the translation t and rotation κ of the collimator from the normal position $\Delta\sigma_t$, $\Delta\sigma_\kappa$ as

$$\Delta\sigma_t\,,\ \Delta\sigma_\kappa = \sigma_x - \sigma - \sigma_c. \tag{25}$$

Figures 9 and 10 show the plotting of $\Delta\sigma_t$ and $\Delta\sigma_\kappa$ against the ratios of t/R_0 and κ/R_0 for various R_0, respec-

Table 1. Conditions used in simulation of X-ray stress measurement for mis-setting and misalignment.

Specimen	Fe		
	Stress σ	(MPa)	-100, 0 and 100
	Half-value breadth HVB	(deg)	2, 4 and 8
Characteristic X-ray and diffraction	CrK_{α} 211		
	Diffraction angle 2θ	(deg)	156.4
	Stress constant K	(MPa/deg)	-318
Measurement method	Ω method (Iso inclination method)		
	Incident angle ψ_0	(deg)	0, 15, 30 and 45
Goniometer	Radius R	(mm)	20~200
	Angle range of PSPC 2α	(deg)	28
Specimen mis-setting	Offset L	(mm)	-2~2
Collimator	Width $2b_{\psi}$	(mm)	1~8
	Effective length Cl	(mm)	150
Collimator misalignment	Translation t	(mm)	-2.5~2.5
	Rotation κ	(deg)	-1.6~1.6

Table 2. Intrinsic stress.

(a) For goniometer radius R_0=200mm

Width $2b_{\psi}$ (mm)	Effective length Cl (mm)	Half-value breadth HVB (deg)		
		2	4	8
0.5	45	-0.5	-0.5	-0.5
	90	-0.2	-0.2	-0.2
	135	-0.1	-0.1	-0.1
1	45	-2.1	-2.0	-1.9
	90	-0.9	-0.9	-0.9
	135	-0.6	-0.6	-0.5
2	45	-9.4	-8.5	-7.9
	90	-3.9	-3.7	-3.5
	135	-2.3	-2.2	-2.1
4	45	-45.4	-37.0	-32.5
	90	-16.9	-15.3	-14.3
	135	-9.5	-9.0	-8.5
8	45	-186.7	-168.1	-132.5
	90	-80.6	-65.7	-58.1
	135	-42.1	-37.2	-34.1

(b) For half-value breadth HVB=2deg

Width $2b_{\psi}$ (mm)	Effective length Cl (mm)	Goniometer radius R_0 (mm)		
		150	200	250
0.5	45	-0.5	-0.5	-0.5
	90	-0.2	-0.2	-0.2
	135	-0.1	-0.1	-0.1
1	45	-2.2	-2.1	-2.1
	90	-0.9	-0.9	-0.9
	135	-0.5	-0.6	-0.6
2	45	-9.8	-9.4	-9.2
	90	-3.9	-3.9	-3.9
	135	-2.1	-2.3	-2.3
4	45	-47.8	-45.4	-43.8
	90	-16.9	-16.9	-16.9
	135	-9.0	-9.5	-9.8
8	45	-199.5	-186.7	-177.7
	90	-80.9	-80.6	-79.7
	135	-39.4	-42.1	-43.3

tively. From these figures, it is seen that the error due to collimator misalignment can be expressed as the following linear relationships as

$$\Delta\sigma_t = -1.1\times10^4 t / R_0, \qquad (26)$$

$$\Delta\sigma_\kappa = 1.7\times10^4 \kappa / R_0. \qquad (27)$$

If the collimator is misaligned under a combination of translation and rotation, the total error $\Delta\sigma_{t\kappa}$ is expressed as

$$\Delta\sigma_{t\kappa} = \Delta\sigma_t + \Delta\sigma_\kappa. \qquad (28)$$

If the stress of mis-set specimen is measured with a misaligned collimator, the error $\Delta\sigma_{Lt\kappa}$ is the total of the errors due to each factor and is expressed as

$$\Delta\sigma_{Lt\kappa} = \Delta\sigma_L + \Delta\sigma_{t\kappa}. \qquad (29)$$

This is seen in Fig. 11, which is the plotting of error versus ratio L/R_0 for various cases of collimator misalignment.

Therefore, the stress value σ_x is estimated by the following equation.

$$\sigma_x = \sigma + \sigma_c + \Delta\sigma_{Lt\kappa}. \qquad (30)$$

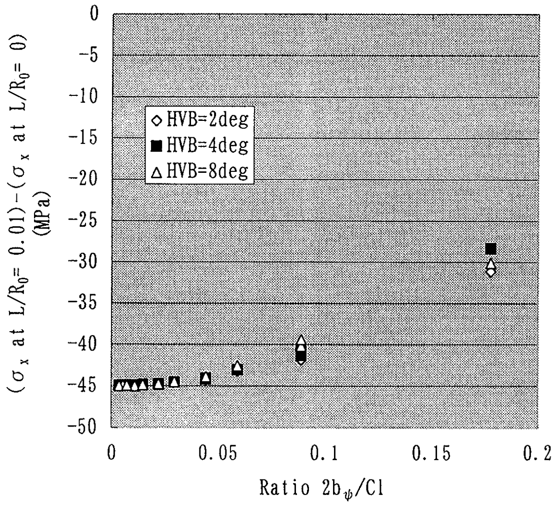

Fig.7. Difference between σ_x at L/R_0= 0.01 and at L/R_0 = 0 versus $2b_\psi/Cl$.

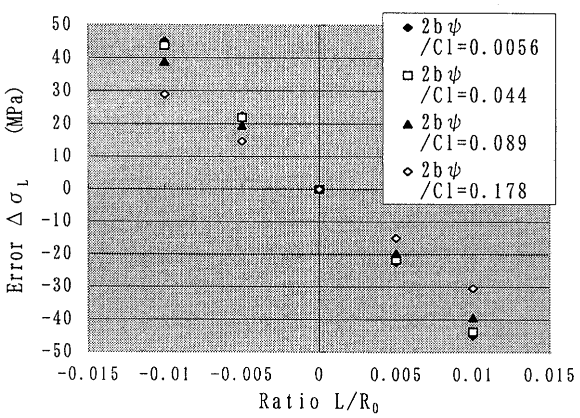

Fig. 8. Error $\Delta\sigma_L$ versus ratio L/R_0.

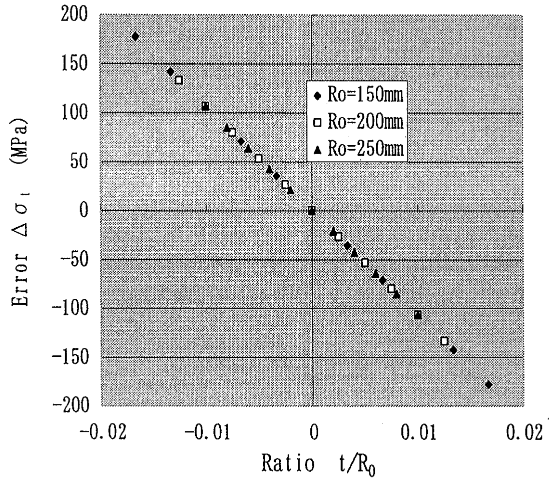

Fig. 9. Error $\Delta\sigma_L$ versus ratio t/R_0.

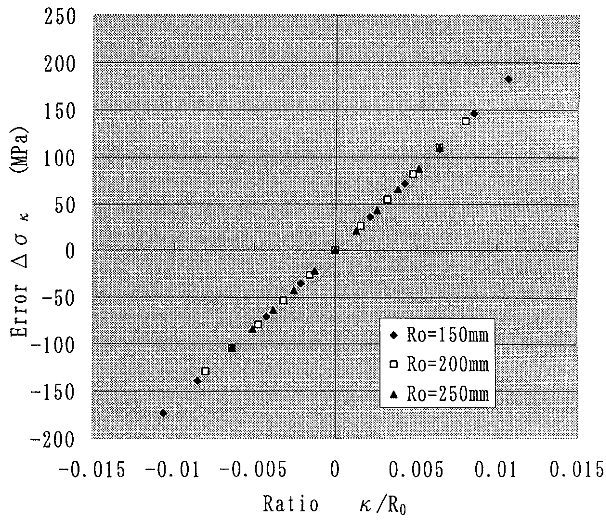

Fig.10. Error $\Delta\sigma_\kappa$ versus ratio κ/R_0.

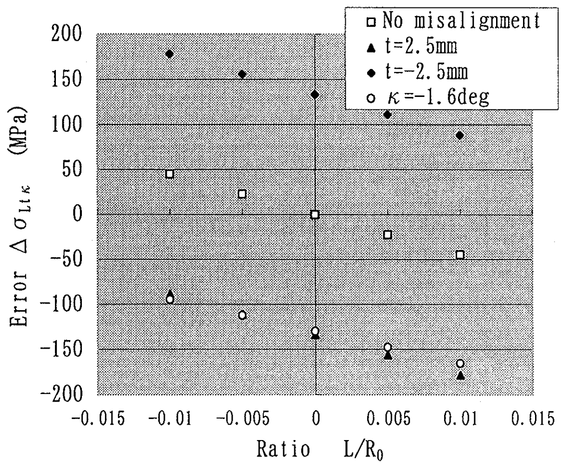

Fig.11. Error $\Delta\sigma_{Lt\kappa}$ versus ratio L/R_0.

4. CONCLUSION

The modeling of X-ray stress measurement using a collimator and a PSPC presented in this study enables us to easily conduct a simulation of the measurement under various conditions for the case of an Ω assembly.

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