Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 24 July 2011
Accepted 13 September 2011

On the polarization state of X-rays generated using a rotating four-quadrant X-ray phase retarder system

Kouhei Okitsu

Nano-Engineering Research Center, Institute of Engineering Innovation, Graduate School of Engineering, The University of Tokyo, 2-11-16 Yayoi, Bunkyo-ku, Tokyo 113-8656, Japan. Correspondence e-mail: okitsu@soyak.t.u-tokyo.ac.jp

A method of calculating the polarization state of X-rays transmitted through a rotating four-quadrant X-ray phase retarder system is described using Jones calculus. This method was applied to correcting the polarization states of X-rays incident on a channel-cut silicon crystal. Details and results of this experiment are given in a separate paper [Okitsu *et al.* (2011), *Acta Cryst.* A**67**, 550–556].

1. Introduction

The transmission-type X-ray phase retarder (Hirano *et al.*, 1991; Giles, Malgrange, Goulon, de Bergevin, Vettier, Dartyge *et al.*, 1994; Giles, Malgrange, Goulon, de Bergevin, Vettier, Fontaine *et al.*, 1994; Hirano *et al.*, 1992, 1993, 1995) opened up a new feasibility to control the polarization state of synchrotron radiation. However, this optical device had problems of phase-shift inhomogeneity owing to the finite angular divergence and energy spread of the incident X-rays, *i.e.* off-axis and chromatic aberrations. The present author and his coauthors developed two-quadrant and four-quadrant phase retarder systems that consist of two and four transmission-type phase retarders, respectively. The former can compensate for off-axis aberration (Okitsu *et al.*, 2001) and the latter can compensate for both off-axis and chromatic aberrations (Okitsu *et al.*, 2002).

Further, the present author and coauthors developed a 'rotating four-quadrant phase retarder system' that can generate arbitrarily polarized X-rays from the horizontally polarized synchrotron X-rays. They also recorded six-beam pinhole topographs for a parallel-plate silicon crystal with arbitrarily polarized X-rays of photon energy 18.245 keV generated with the phase retarder system. The experimentally obtained pinhole topographs for a parallel-plate silicon crystal were quantitatively in good agreement with computer-simulated ones based on the *n*-beam Takagi–Taupin equation (Okitsu *et al.*, 2006; hereafter denoted O *et al.* 2006). More recently, they have reported qualitative and quantitative agreements between experimentally obtained and computer-simulated pinhole topographs for a channel-cut silicon crystal (Okitsu *et al.*, 2011; hereafter denoted O *et al.* 2011). However, the photon energy used in the experiment was 18.475 keV which was slightly different from that used in the case of the parallel-plate crystal. The angular positions of the phase retarder crystals were values obtained for 18.245 keV (O *et al.* 2006). It was then necessary to obtain the correct polarization states used in the experiment for the channel-cut silicon crystal at 18.475 keV. The following section describes the method of calculating the polarization states based on Jones calculus.

2. Correction for the polarization states of X-rays generated by the phase retarder system

The change of polarization state can be described using Jones calculus (Jones, 1941) in general. The amplitude vector whose original polarization state is horizontal is represented by a Jones vector, $\mathbf{D}_0 = (D_0^{(h)}, D_0^{(v)}) = (1, 0)$. Here, $D_0^{(h)}$ and $D_0^{(v)}$ are the complex amplitudes of X-rays for which the directions of polarization are horizontal and vertical, respectively. $\mathbf{D}_0$ is transformed to $\mathbf{D}_0'$ by transmission through the four-quadrant phase retarder system (Okitsu *et al.*, 2002) as follows,

$$\mathbf{D}_0' = \mathbf{R}\Psi\mathbf{R}^{-1}\mathbf{D}_0, \tag{1}$$

where

$$\mathbf{R} = \begin{bmatrix} \cos(45^\circ + \chi_{\rm PR}) & -\sin(45^\circ + \chi_{\rm PR}) \\ \sin(45^\circ + \chi_{\rm PR}) & \cos(45^\circ + \chi_{\rm PR}) \end{bmatrix}, \tag{2}$$

$$\mathbf{\Phi} = \begin{bmatrix} \exp(-i\Delta\varphi_{\rm total}/2) & 0 \\ 0 & \exp(i\Delta\varphi_{\rm total}/2) \end{bmatrix}. \tag{3}$$

Here, $\chi_{\rm PR}$ is the rotation angle of the phase retarder system and $\Delta\varphi_{\rm total}$ is the total phase shift given by the phase retarder system, as defined by O *et al.* 2006. Hereafter, amplitude vectors are column vectors in the matrix calculations whereas they are described as raw vectors in the text.

On the other hand, $\mathbf{D}_0'$ can necessarily be written as a linear combination of left- and right-screwed circular polarizations whose complex amplitude vector $\mathbf{D}_0'^{(\rm LR)} = (D_0'^{(\rm L)}, D_0'^{(\rm R)})$ as follows,

$$\mathbf{D}_0' = \frac{D_0'^{(\rm L)}}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} + \frac{D_0'^{(\rm R)}}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}.$$

Therefore,

$$\mathbf{D}_0' = \mathbf{M}_{\rm C}\mathbf{D}_0'^{(\rm LR)}, \quad \text{where} \quad \mathbf{M}_{\rm C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}. \tag{4}$$

By substituting (1) into (4), $\mathbf{D}_0^{\prime(\mathrm{LR})}$ can be obtained by

$$\mathbf{D}_0^{\prime(\mathrm{LR})} = \mathbf{M}_\mathrm{C}^{-1}\mathbf{R}\mathbf{R}^{-1}\mathbf{D}_0. \tag{5}$$

Because the lengths of the major and minor axes of the elliptical polarization $\mathbf{D}_0^{\prime(\mathrm{LR})}$ are $2(|D_0^{\prime(\mathrm{L})}| + |D_0^{\prime(\mathrm{R})}|)$ and $2(|D_0^{\prime(\mathrm{L})}| - |D_0^{\prime(\mathrm{R})}|)$, the ellipticity R is given by

$$R = \frac{\left|D_0^{\prime(\mathrm{L})}\right| - \left|D_0^{\prime(\mathrm{R})}\right|}{\left|D_0^{\prime(\mathrm{L})}\right| + \left|D_0^{\prime(\mathrm{R})}\right|}, \tag{6}$$

where the sign of R is positive when the polarization is left-screwed. Further, the directions of the electric field vectors of left- and right-screwed circular polarizations described as $D_0^{\prime(\mathrm{L})}(1, -i)/\sqrt{2}$ and $D_0^{\prime(\mathrm{R})}(1, i)/\sqrt{2}$ are inclined by $\arg(D_0^{\prime(\mathrm{L})})$ and $-\arg(D_0^{\prime(\mathrm{R})})$, respectively, viewed from the downstream direction when $\nu t - \mathbf{K}_0 \cdot \mathbf{r} = 0$, because the rotation helicities are contrary between the left- and right-screwed circular polarizations. Here, the amplitudes of X-rays with left- and right-screwed circular polarizations are assumed to be represented by $D_0^{\prime(\mathrm{L})}\exp[\mathrm{i}2\pi(\nu t - \mathbf{K}_0 \cdot \mathbf{r})]$ and $D_0^{\prime(\mathrm{R})}\exp[\mathrm{i}2\pi(\nu t - \mathbf{K}_0 \cdot \mathbf{r})]$, where ν and $\mathbf{K}_0$ are the frequency and wavevector of incident X-rays, t is the time and $\mathbf{r}$ is the location vector. The directions of the electric field vectors of these circular polarizations are inclined by the same angle $[\arg(D_0^{\prime(\mathrm{L})}) - \arg(D_0^{\prime(\mathrm{R})})]/2$ from the horizontal plane when $2\pi(\nu t - \mathbf{K}_0 \cdot \mathbf{r}) = -[\arg(D_0^{\prime(\mathrm{L})}) + \arg(D_0^{\prime(\mathrm{R})})]/2$. Therefore, the inclined angle of the major axis of the elliptical polarization χ_MA is given by

$$\chi_\mathrm{MA} = \left[\arg(D_0^{\prime(\mathrm{L})}) - \arg(D_0^{\prime(\mathrm{R})})\right]/2. \tag{7}$$

When χ_PR and $\Delta\theta_{\mathrm{PR}_n}$ were controlled as summarized in Table 3 of O *et al.* 2006 at the photon energy of 18.245 keV, LH, LV, L-45° and CL polarizations were generated. In the experiment of O *et al.* 2011, however, values of χ_PR and $\Delta\theta_{\mathrm{PR}_n}$ summarized in Table 2 of O *et al.* 2011, obtained from the experimental result shown in Fig. 6 of O *et al.* 2006, were used by mistake in spite of the slightly different photon energy.

Incidentally, according to Hirano *et al.* (1995), the σ–π phase shift $\Delta\varphi_\mathrm{PR}$ given by the transmission-type X-ray phase retarder is approximately described as follows,

$$\Delta\varphi_\mathrm{PR} = -\frac{\pi z f(E)}{2\Delta\theta_\mathrm{PR}}, \quad \text{where} \quad f(E) = \frac{\left|\chi_h^{(\mathrm{R})}\right|^2 \sin(2\theta_\mathrm{B})}{\lambda\cos(\alpha)}. \tag{8}$$

Here, z is the thickness of the transmission-type phase retarder crystal, $\Delta\theta_\mathrm{PR}$ is the angular deviation from the exact Bragg condition of the phase retarder whose reflection vector is $\mathbf{h}$, $\chi_h^{(\mathrm{R})}$ is the real part of the $\mathbf{h}$th-order Fourier coefficient of electric susceptibility of the phase retarder crystal, θ_B is the Bragg reflection angle of the phase retarder, λ is the wavelength of the X-rays and α is the angle spanned by the direction of X-ray transmission and the downstream normal of the surface of the phase retarder crystal. $f(E)$ is a term depending on the photon energy of the X-rays.

Values of $\Delta\theta_{\mathrm{PR}_n}$ ($n \in \{1, 2, 3, 4\}$) that had absolute values of the position (*b*) and signs (*c*) shown in Fig. 6 of O *et al.* 2006 were used by mistake for intending to generate LV and L-45° polarizations. Furthermore, the absolute values (*a*) and signs (*d*) were used for intending to generate CL polarization. First, it was assumed that the position (*c*) and (*d*) in Fig. 6 of O *et al.* 2006 gave the total phase-shift values $\Delta\varphi_\mathrm{total}$ of π and $\pi/2$, respectively, at 18.245 keV. Then, values of $\Delta\varphi_\mathrm{total}$ at 18.245 keV at angular positions summarized in Table 2 of O *et al.*, 2011 for LV, L-45° and CL were estimated based on equation (8) with $f(E) = f[18.245\,(\mathrm{keV})]$. Further, these phase-shift values were multiplied by $f[18.475\,(\mathrm{keV})]/f[18.245\,(\mathrm{keV})]$, which was calculated to be 0.9494301, to obtain the phase-shift values at 18.475 keV. Values of $\Delta\varphi_\mathrm{total}$ shown in Table 2 of O *et al.* 2011 were evaluated based on the above procedure. Substituting these values of $\Delta\varphi_\mathrm{total}$ and χ_PR into (2) and (3), the Jones vectors $\mathbf{D}_0'$ were calculated using (1). $\mathbf{D}_0'$ were transformed to $\mathbf{D}_0^{\prime(\mathrm{LR})}$ using (5). The ellipticity R and the inclined angle χ_MA were calculated using (6) and (7) as summarized in Table 2 of O *et al.* 2011.

With regard to LH polarization, values of $\Delta\theta_{\mathrm{PR}_n}$ were controlled such that $\Delta\varphi_\mathrm{total}$ calculated using equation (10) of O *et al.* 2006 was zero to generate LH polarization in O *et al.* 2011. However, the value of $\Delta\varphi_\mathrm{total}$ for intending to generate LH polarization in O *et al.* 2006 can be calculated to be 0.0580π, which means generation of a left-screwed elliptical polarization with an ellipticity of 0.0913 that can be calculated by $R = \tan(\Delta\varphi_\mathrm{total}/2)$ using equations (1)–(3), but not an exactly horizontal-linear polarization. When intending to generate horizontal-linearly polarized X-rays, the condition $\Delta\varphi_\mathrm{total} = 0$ is more important than the condition given by equation (9) of O *et al.* 2006.

The values of R and χ_MA summarized in Table 2 of O *et al.* 2011 were used for obtaining the computer-simulated topographs in that paper.

The present work was performed at the High-Power X-ray Laboratory, Nano-Engineering Research Center, Institute of Engineering Innovation, Graduate School of Engineering, The University of Tokyo, Japan. Practical calculations of polarization state of X-rays based on the present work were performed using the facilities of the Supercomputer Center, Institute for Solid State Physics, The University of Tokyo, Japan. The present work is one of the activities of the Active Nano-Characterization and Technology Project financially supported by the Special Coordination Fund of the Ministry of Education, Culture, Sports, Science and Technology of the Japanese government.

References

Giles, C., Malgrange, C., Goulon, J., de Bergevin, F., Vettier, C., Dartyge, E., Fontaine, A., Giorgetti, C. & Pizzini, S. (1994*a*). *J. Appl. Cryst.* **27**, 232–240.
Giles, C., Malgrange, C., Goulon, J., de Bergevin, F., Vettier, C., Fontaine, A., Dartyge, E. & Pizzini, S. (1994*b*). *Nucl. Instrum. Methods Phys. Res. A*, **349**, 622–625.
Hirano, K., Ishikawa, T. & Kikuta, S. (1993). *Nucl. Instrum. Methods Phys. Res. A*, **336**, 343–353.
Hirano, K., Ishikawa, T. & Kikuta, S. (1995). *Rev. Sci. Instrum.* **66**, 1604–1609.
Hirano, K., Ishikawa, T., Koreeda, S., Fuchigami, K., Kanzaki, K. & Kikuta, S. (1992). *Jpn. J. Appl. Phys.* **31**, L1209–L1211.
Hirano, K., Izumi, K., Ishikawa, T., Annaka, S. & Kikuta, S. (1991). *Jpn. J. Appl. Phys.* **30**, L407–L410.
Jones, R. C. (1941). *J. Opt. Soc. Am.* **31**, 488–493.
Okitsu, K., Ueji, Y., Sato, K. & Amemiya, Y. (2001). *J. Synchrotron Rad.* **8**, 33–37.
Okitsu, K., Ueji, Y., Sato, K. & Amemiya, Y. (2002). *Acta Cryst.* A**58**, 146–154.
Okitsu, K., Yoda, Y., Imai, Y. & Ueji, Y. (2011). *Acta Cryst.* A**67**, 550–556.
Okitsu, K., Yoda, Y., Imai, Y., Ueji, Y., Urano, Y. & Zhang, X. (2006). *Acta Cryst.* A**62**, 237–247.