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X-ray diffraction with a Bragg angle near $\pi/2$ and its applications

S. Kikuta,[a*] Y. Imai,[a] T. Iizuka,[a] Y. Yoda,[a] X.-W. Zhang[b] and K. Hirano[b]

[a]*Department of Applied Physics, School of Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan, and [b]Photon Factory, High Energy Accelerator Research Organization, Oho, Tsukuba-shi, Ibaraki 305, Japan. E-mail: kikuta@kohsai.t.u-tokyo.ac.jp*

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X-ray dynamical diffraction phenomena at a Bragg angle near $\pi/2$ are studied. The X-ray transmissivity as well as the reflectivity from the (991) lattice plane of a silicon thin plate is observed. It agrees fairly well with the diffraction pattern calculated on the basis of the Darwin approach. The possibility is discussed whether a set of two crystal plates arranged face to face, in which the diffraction condition with a Bragg angle near $\pi/2$ is satisfied, may be used as a very high resolution monochromator.

Keywords: X-ray crystal components; $\pi/2$ Bragg angle; dynamical diffraction phenomena; very high resolution monochromators.

1. Introduction

Dynamical diffraction phenomena of X-rays at a Bragg angle near $\pi/2$ have been studied before. Kohra & Matsushita (1972) first studied these phenomena. It has been shown that the half-width of a diffraction pattern at a Bragg angle near $\pi/2$ is about 10^3 times as broad as that for the usual case. Detailed studies have been made by Brümmer *et al.* (1979) and Caticha & Caticha-Elis (1982). In these studies the fomulation of the dynamical diffraction theory of von Laue was used, which consists of solving Maxwell's equations in a continuous periodic medium. Graeff & Materlik (1982) have demonstrated that Bragg backscattering resolves energy in the meV range. Colella & Luccio (1984) have proposed an application to a new type of X-ray resonator.

So far in dynamical diffraction at a Bragg angle near $\pi/2$, the reflectivity has been mainly treated. In this report we observe the transmissivity from a silicon crystal plate in addition to the reflectivity, and compare it with calculated values. As an application of an X-ray crystal component with a Bragg angle of $\pi/2$, the possibility of use as a monochromator with a very high resolution is discussed.

2. Transmissivity and reflectivity from a silicon crystal plate at a Bragg angle near $\pi/2$

The experiment was performed at BL15C of the Photon Factory. Fig. 1 shows the experimental arrangement. Synchrotron radiation is highly monochromated and collimated by a high-resolution monochromator. It is composed of two channel-cut silicon crystals with symmetric (777) reflections arranged in the dispersive setting. For observing the diffraction pattern for a Bragg angle near $\pi/2$, a silicon crystal plate specimen with the (991) reflection was used. The surface of the specimen crystal was parallel to the (991) lattice plane. The X-ray wavelength relevant to this reflection was about 0.8508 Å. In front of the specimen, a forecrystal of a silicon plate with symmetric Laue-case (220) diffraction was arranged. The X-ray beam was diffracted from the forecrystal and then incident on the specimen. The transmissivity from the specimen was measured by rotating the specimen around the normal position. The reflected beam from the specimen was transmitted through the forecrystal. The reflectivity from the specimen was measured in front of the forecrystal. The observed transmissivity curve and reflectivity curve are shown in Fig. 2(a). In this case the thickness of the specimen crystal is 226 µm. The transmissivity curve has a large dip with a width of about 256 arcsec. The reflectivity curve has a broad peak with a width of about 234 arcsec. In the reflec-

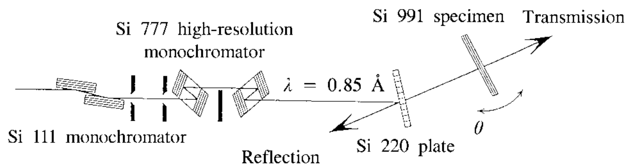

Figure 1
Experimental arrangement for observing the X-ray transmissivity and reflectivity curves from a silicon crystal plate at a Bragg angle near $\pi/2$.

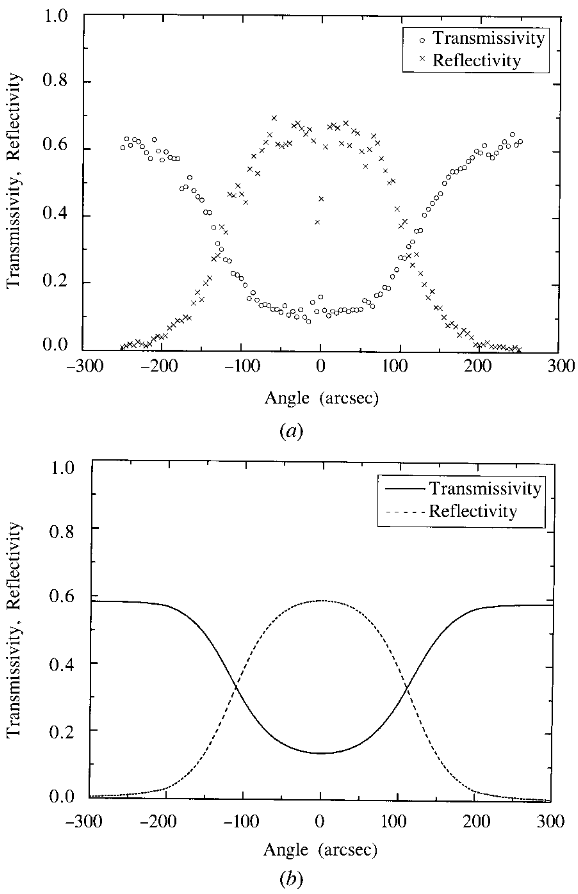

Figure 2
Transmissivity and reflectivity curves from a 226 µm-thick silicon crystal plate for the 991 reflection at a Bragg angle near $\pi/2$. (a) Observed curves; (b) calculated curves. A rotation angle is represented as the deviation from $\pi/2$.

tivity curve there is a sharp dip at the exact Bragg angle of $\pi/2$. It is attributed to multiple reflections of $(40\bar{4})$, $(04\bar{4})$, (955) and (595) which occur simultaneously at normal incidence to the (991) plane.

The calculation of the diffraction pattern was made by using the formulation of the dynamical diffraction theory of Darwin. This formulation has recently been developed by Nakatani & Takahashi (1994). In the Darwin theory the crystal is regarded as a periodic stack of atomic layers consisting of several atomic planes. X-rays are reflected repeatedly from each atomic layer of the crystal. The relations between the transmission amplitude and the reflection amplitude among the layers are given in the form of recursion formulae called the Darwin difference equations. The transmissivity and reflectivity from the whole crystal can be obtained by using the mathematical techniques of optical thin-film theory. Fig. 2(*b*) shows the calculated transmissivity and reflectivity curves corresponding to those in Fig. 2(*a*). In the calculation, the intrinsic curves were convoluted with the energy spread and the angular spread from the high-energy-resolution monochromator. In the case of the reflectivity curve, the X-ray attenuation in the forecrystal was taken into account. The dip width of the transmissivity curve and peak width of the reflectivity curve are both 234 arcsec. The profiles of the observed diffraction patterns agree fairly well with those of the calculated ones.

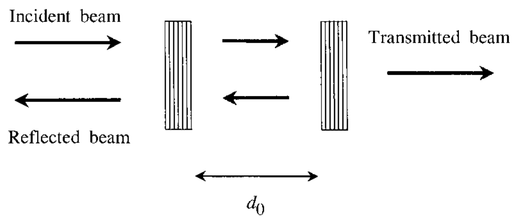

Figure 3
X-ray crystal component composed of two crystal plates arranged face to face with a gap width d_0. An incident beam is diffracted by a lattice plane parallel to the crystal surface with a Bragg angle near $\pi/2$.

3. Application of X-ray crystal component with a Bragg angle of $\pi/2$

Now we consider the case where two crystal plates are arranged face to face instead of one crystal plate, as shown in Fig. 3. The transmissivity and reflectivity from a set of two crystal plates were calculated as functions of the width between the two plates and the angular deviation from the normal position on the basis of the dynamical diffraction theory of Darwin as before, as shown in Fig. 4. Here, the (0016) reflection of silicon was used for the diffraction condition of a Bragg angle near $\pi/2$. The X-ray wavelength which satisfies the diffraction condition at normal incidence was used. It

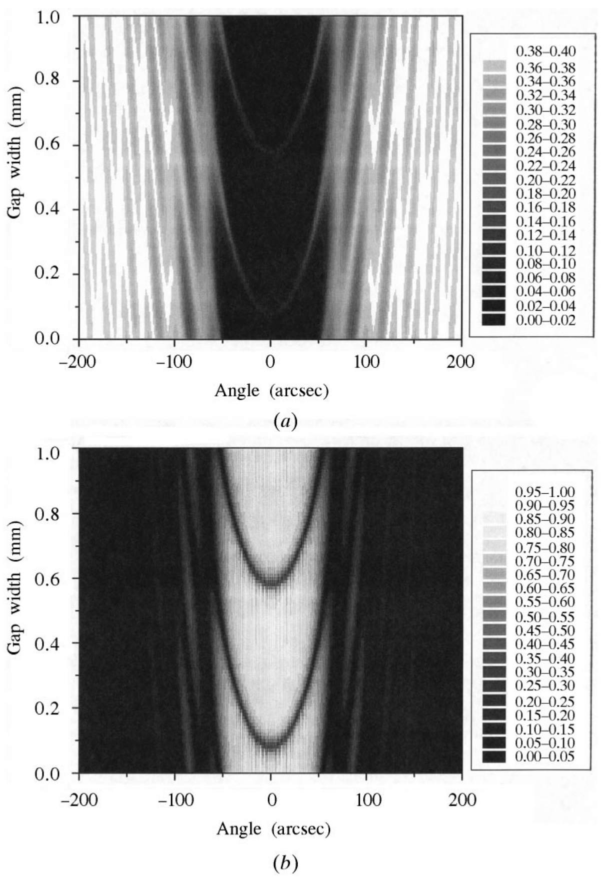

Figure 4
Calculated contour maps of the transmissivity (*a*) and reflectivity (*b*) from a set of two crystal plates at a Bragg angle near $\pi/2$ represented as functions of the incident angle and the gap width between two crystal plates. The (0016) reflection of silicon is used. The X-ray wavelength relevant to this reflection is about 0.6789 Å. The thickness of each plate is 0.4 mm and the gap width is changed from d_0 ($\simeq$ 0.5 mm), where d_0 is assumed to be an exact multiple of d_{0016}, the (0016) lattice spacing, to $d_0 + 2d_{0016}$. The angle 0 arcsec corresponds to the position of normal incidence. White regions indicate high X-ray intensity.

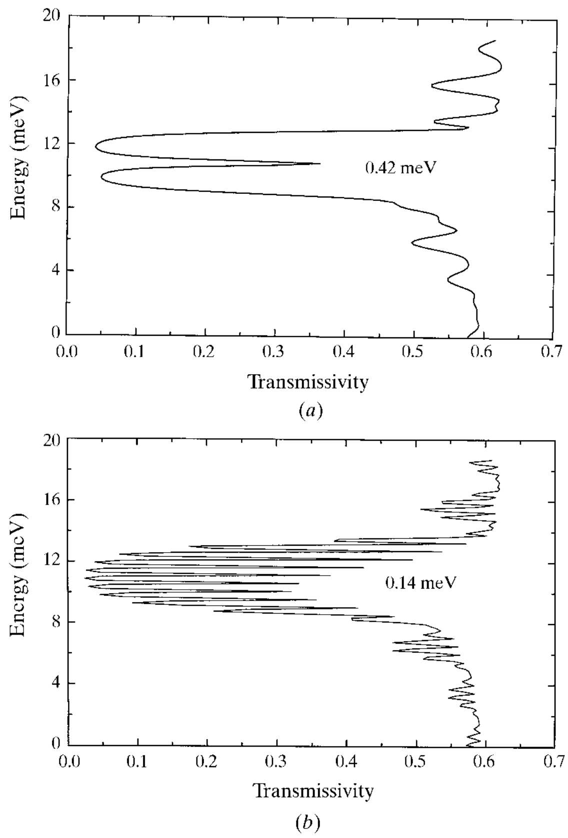

Figure 5
Calculated transmissivity of the (0016) reflection from a set of two crystal plates as a function of X-ray energy. The change in a very small energy range at about 18.26 keV is shown. The thickness of each crystal plate is 200 μm. The gap width is 100 μm in (*a*) and 1 mm in (*b*).

is assumed that two plates have a thickness of 0.4 mm. The gap width between two plates is $d_0 \simeq 0.5$ mm, where d_0 is assumed to be an exact multiple of d_{0016}, the (0016) lattice spacing. In Fig. 4 the gap width is changed from d_0 to $d_0 + 2d_{0016}$. In the transmissivity and reflectivity curves, sharp peaks and sharp dips are seen inside the angular range of Bragg reflection, respectively. These are caused by multiple interference among many reflected and transmitted beams from two crystal plates.

The change in the transmissivity from a set of two crystal plates for the (0016) reflection with X-ray energy was calculated. Figs. 5(a) and 5(b) show the cases where the gap width is 100 µm and 1 mm, respectively, with a plate thickness of 200 µm. When the gap width is equal to a multiple of half a wavelength, the waves reflected forwards and backwards in the gap interfere constructively. As a result a standing wave is formed. As shown in Fig. 5, in the case of a narrow gap width, only a single line appears within the range of Bragg reflection. In the case of the broader gap width, many lines with smaller energy width appear. A monolithic set of two crystal plates analogous to the optical Fabry–Perot etalon may be applied as a high-resolution monochromator, as proposed by Steyerl & Steinhauser (1979). They suggested filling the gap with an appropriate immersion liquid so that the wavelength in the liquid is equal to twice the lattice spacing. Another method of adjusting the optical path length is to set a phase object in the gap in the case of the wide gap.

To suppress the forward-scattered beam outside the range of Bragg reflection in the set of two crystal plates, a pre-monochromator is needed which provides a narrow bandwidth. It may be possible to obtain an extremely highly monochromatic beam with an energy band near 0.1 meV by arranging two sets of two crystal plates in tandem. In this case the gap width of the second set is chosen to be narrower than that of the first set.

4. Conclusions

The X-ray transmissivity as well as reflectivity from a thin crystal plate at a Bragg angle near $\pi/2$ was studied. Diffraction phenomena in the case of a set of two crystal plates were also analysed by simulation. It was recognized that the dynamical theory of Darwin was suitable for the numerical calculations in these studies.

Although the transmissivity curve for a thin crystal plate has a broad dip expressed in the energy range as well as in the angular range of Bragg reflection, in the case of two crystal plates sharp lines with narrow energy width appear in a broad dip expressed in the energy range owing to the multiple interference effect. A very high resolution monochromator providing a narrow energy band of about 0.1 meV may be realizable by a combination of several crystal plates.

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