The Effect of Crystal Dispersion on the X-ray Emission Spectrum Observed using a Double Crystal Spectrometer

Tatsunori Tochio, Yoshiaki Ito and Kazuhiko Omote

The effect of the rocking curve on the x-ray emission spectrum observed using a double-crystal spectrometer was discussed. The results for Si (220) crystal at 1.54056Å (Cu Kα_1) show that the x-ray of wavelength λ_0-$\Delta\lambda$ ($\Delta\lambda$=0.00007Å) is much more reflected by the double crystal put in the (++) position of θ_B than the x-ray of wavelength λ_0 which exactly satisfies the Bragg condition. In the last we mentioned what we observe in our measurement with a double-crystal spectrometer.

Keywords: double-crystal spectrometer/ rocking curve/ x-ray emission spectrum

X-ray emission spectroscopy is known as a valuable tool for estimating the level width and the probabilities of various multi-electron transitions. In spite of its usefulness the instrumental function which is specific for the spectrometer used makes a precise analysis difficult. The instrumental function for a double-crystal spectrometer is relatively small compared with that for a single crystal spectrometer because the first crystal plays the same role as a narrow slit. But even for a double crystal spectrometer the instrumental function cannot be neglected. The aim of our work is to evaluate the effect of the crystal dispersion on the x-ray emission spectrum observed by means of a double-crystal spectrometer and to establish the way to analyze it. The crystal dispersion is considered to be a main component of the instrumental function in a double-crystal spectrometer and we may assume that the contributions from other components are almost negligible.

First we consider the monochromatic x-ray which has the wavelength λ_0 satisfying the Bragg condition with the Bragg angle θ_B determined by the positions of two crystals. As can be seen from the Figure1, the beam reflected on the first crystal by the angle of $\theta=\theta_B+d\theta$ makes an incidence angle of $\theta'=\theta_B-d\theta$ with the surface of the second crystal. This gives us the expression for the rocking curve for double crystal ($R_D(\theta_B;\lambda_0;\theta')= R_D(\theta_B;\lambda_0;2\theta_B-\theta)$) as follows.

$$R_D(\theta_B;\lambda_0;\theta')=R_S(\theta_B;\lambda_0;\theta')\times R_S(\theta_B;\lambda_0;2\theta_B-\theta'). \quad (1)$$

Here, $R_S(\theta)$ expresses the rocking curve for single crys-

STATES AND STRUCTURES — Atomic and Molecular Physics —

Scope of Research

In order to obtain fundamental information on the property and structure of materials, the electronic states of atoms and molecules are investigated in detail using X-ray, SR, ion beam from accelerator and nuclear radiation from radioisotopes. Theoretical analysis of the electronic states and development of new radiation detectors are also performed.

Assoc. Prof
ITO,
Yoshiaki
(D Sc)

Instructor
KATANO,
Rintaro
(D Eng)

Instructor
NAKAMATSU,
Hirohide
(D Sc)

students:
SHIGEMI, Akio (DC)
TOCHIO, Tatsunori (DC)
MASAOKA, Sei (DC)
SHIGEOKA, Nobuyuki (DC)
MUTAGUCHI, Kohei (MC)
OHASHI, Hirofumi (MC)
NAKANISHI, Yoshikazu (RF)

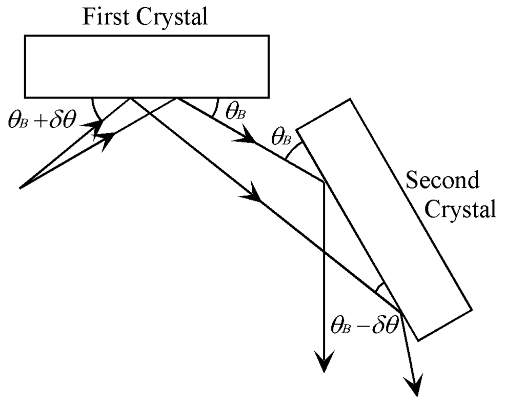

Figure1. Schematic diagram of the reflections by double-crystal with (++) position

tal which we define as the average of the rocking curve for the normal polarization and that for the parallel polarization. In the normal polarization the electric vector $\boldsymbol{E}$, at the moment when the x-ray is reflected, is normal to the plane containing the wave vector for the incident beam $\boldsymbol{k}_0$ and that for the diffracted beam $\boldsymbol{k}_H$, while in the parallel polarization the electric vector $\boldsymbol{E}$ lies in that plane. The curves of $R_D(\theta') = R_D(2\theta_B - \theta)$ for Si(220) at Cu Kα_1 energy are shown in the Figure 2- (a).

Now we consider the beam having the wavelength λ' which is very close to λ_0. The Bragg angle for this beam θ_B' is given by

$$\theta_B' \cong \theta_B + \left(\frac{d\theta}{d\lambda}\right)_{\lambda=\lambda_0}(\lambda'-\lambda_0) = \theta_B + \frac{\lambda'-\lambda_0}{\lambda_0}\tan\theta_B \qquad (2)$$

This leads to the expression for the rocking curve in a double-crystal (The attention should be paid to the fact that the positions of the two crystals are not for θ_B' but for θ_B.) at the wavelength of λ' as follows.

$$\begin{aligned} R_D(\theta_B;\lambda';\theta') &= R_S(\theta_B;\lambda';\theta') \times R_S(\theta_B;\lambda';2\theta_B-\theta') \\ &\cong R_S\left(\theta_B;\lambda_0;\theta' - \frac{\lambda'-\lambda_0}{\lambda_0}\tan\theta_B\right) \\ &\quad \times R_S\left(\theta_B;\lambda_0;2\theta_B-\theta' + \frac{\lambda'-\lambda_0}{\lambda_0}\tan\theta_B\right). \end{aligned} \qquad (3)$$

We can easily check that $R_D(\theta_B;\lambda';\theta)$ corresponds to equation (1) when λ' is equal to λ_0. For $\lambda' = \lambda_0 - \Delta\lambda$, $\lambda_0 + \Delta\lambda$ ($\Delta\lambda = 0.00007$ Å), the curve of $R_D(x;\theta)$ is shown in the Figure 2-(b),(c) respectively. Figure 2- (a),(b),(c) show that the x-ray of wavelength $\lambda_0 - \Delta\lambda$ is reflected most strongly compared with the others. In fact *S(a)* : *S(b)* : *S(c)*, the ratio of the area under the curve, is approximately 4 : 67 : 1. When the intensity distribution of the incident beam on the wavelength λ is $I_{in}(\lambda)$, the intensity distribution of the diffracted beam becomes

$$I_{out}(\theta_B;\lambda) = \int I_{in}(\lambda) R_D(\theta_B;\lambda;\theta')\,d\theta'. \qquad (4)$$

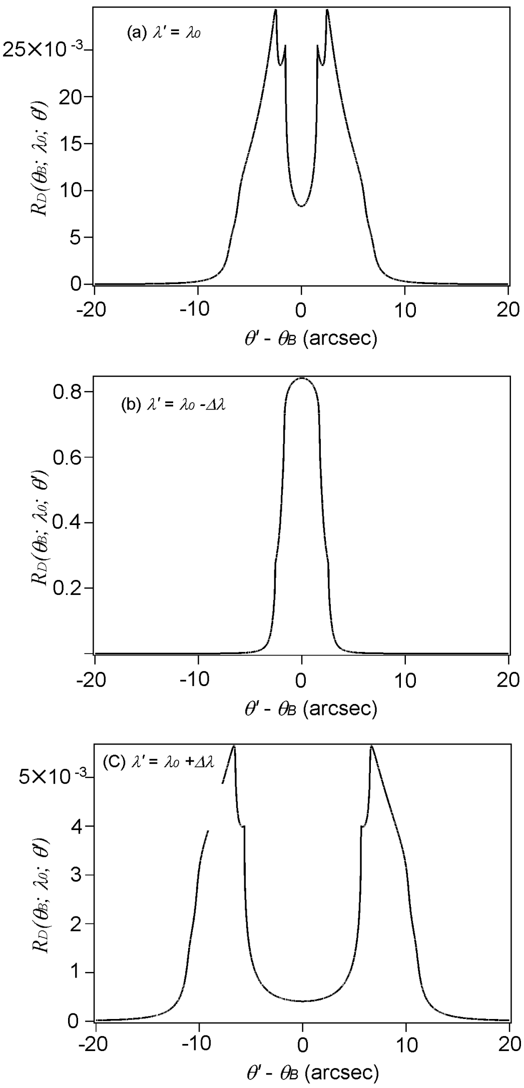

Figure 2. $R_D(\theta_B;\lambda';\theta')$ for Si (220) at (a) $\lambda' = \lambda_0$ (λ_0 =1.54056**Å**), (b) $\lambda' = \lambda_0 - \Delta\lambda$ ($\Delta\lambda$=0.00007 **Å**), (c) $\lambda' = \lambda_0 + \Delta\lambda$ ($\Delta\lambda$=0.00007 **Å**)

Inversely, the the intensity distribution of the diffracted beam in the direction θ' is expressed as follows .

$$I_{out}(\theta_B;\theta') = \int I_{in}(\lambda) R_D(\theta_B;\lambda;\theta')\,d\lambda. \qquad (5)$$

The range of angle or wavelength having a significant intensity is so small that the detector can count all the photons in this range. Then the expression for what we observe is written as

$$I_{out}(\theta_B) = \iint I_{in}(\lambda) R_D(\theta_B;\lambda;\theta')\,d\lambda\,d\theta' \qquad (6)$$

The observed spectrum is considered to be the trace of $I_{out}(\theta_B)$ at each point of θ_B which we change during the scan.