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

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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.

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

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.

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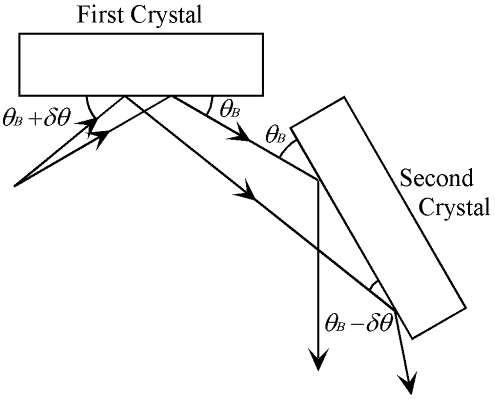

Figure1. Schematic diagram of the reflections by double-crystal with (++) position

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 λ_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

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

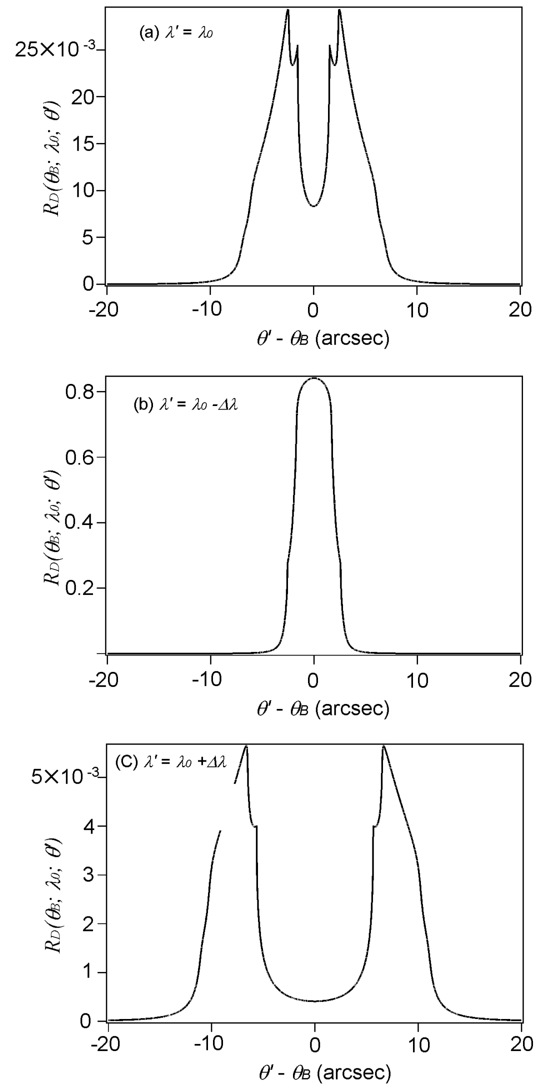

Figure 2. $R_D(\theta_B; \lambda';\theta')$ for Si (220) at (a) $\lambda'= \lambda_0$ (λ_0 =1.54056**Å**), (b) $\lambda' = \lambda_0$-$\Delta\lambda$ ($\Delta\lambda$=0.00007 **Å**), (c) $\lambda'= \lambda_0$+$\Delta\lambda$ ($\Delta\lambda$=0.00007 **Å**)

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.