# X-ray standing wave study on the impurities in calcium fluoride single crystal

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## **Introduction**

The calcium fluoride  $(CaF_2)$  is an attractive material for the ultraviolet optics by reason of its high transparence for the light. Impurities in CaF<sub>2</sub> could cause decrease of the penetrating power of the light and yield fluorescence, even if their quantities were very small. Not only the species of impurities and their quantities but also the position in the CaF<sub>2</sub> lattice is very important to clear up the mechanisms of these problems. In this study we examined the several impurities in the CaF<sub>2</sub> single crystal to clear their crystallographic position by using X-ray standing wave technique<sup>1</sup>.

#### **Experimental**

Experiments were performed at BL4A. The schematic illustration of the measurement system is shown in Figure 1. The X-ray beam from the storage ring was monochromated to 18.5keV by the Si (111) double crystal monochromator. The monochromated X-rays were formed to 1.0mm (horizontal)  $\times$  0.2mm (vertical) by the slits. Two ionization chambers were used to detect the X-rays. One of them detected the incident intensity of X-rays and the other detected diffracted X-ray intensity. The X-ray fluorescence from impurities was detected by the Si (Li) solid-state detector (SSD).



Fig. 1. The schematic illustration of experimental system at BL4A.

The CaF<sub>2</sub> ingot was grown by the Bridgman-Stockbarger method using natural calcium fluoride as the raw material. The species and quantities of the impurities in the CaF<sub>2</sub> were determined by inductively coupled plasma mass spectrometry (ICP-MS). There were some alkaline earth elements and rare earth elements in the CaF<sub>2</sub> and the concentrations of them were less than 100ppm. The sample crystal was cut down 10mm × 10mm × 5.0mm with <111>surface normal from the ingot. The intensities of the X-ray fluorescence from the calcium and impurities were recorded while stepping up in angle through the symmetric (111) reflection.

## **Results and Discussion**

The rocking curve profile and the intensity of X-ray fluorescence of Sr K  $\alpha$  were shown in figure 2. The intensity of X-ray fluorescence in the standing wave field<sup>2</sup> is given by

$$Y \propto 1 + R + 2\sqrt{R} f_c \cos(\nu - 2\pi P_c).$$
(1)

*R* is the X-ray reflectivity. v is the value of phase of the reflected wave.  $f_c$  and  $P_c$  are the coherent fraction and the coherent position. To find the best value of  $f_c$  and  $P_c$ , the experimental data were fitted by equation (1). The value of the coherent position  $P_c = d_{Sr} / d_{111}$  and the coherent fraction  $f_c$  are equal to 0.80 and 0.93.



Fig. 2. XSW results in the case of Sr K  $\alpha$ . The solid circle represents the observed reflectivity of the (111) Bragg reflection. The open circle represents the normalized intensity of X-ray fluorescence. The solid lines are calculated intensities of Bragg reflection and X-ray fluorescence.

Using XSW technique, we enabled to obtain that the crystallographic positions of the impurities in the  $CaF_2$ . We are going to consider relationships between these information and the optical properties.

# **References**

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