Structure Investigation of Ca₂CoSi₂O₇

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Introduction

Weissenberg photography method is useful for investigations of intensity distribution in reciprocal space, in particular under specific condition such as high pressure, high or low temperatures. The beam line 1B at Photon Factory is suitably designed for such experiments: the attachments for high pressure, low and high temperatures are connected with the Weissenberg system with Imaging Plate (IP) detector. The method is also effective for the observation of intensity variation due to the anomalous dispersion effects those are realized by scanning of incident X-ray energy around absorption edge of the specific chemical element. In the present experiment, we aim to measure the intensity distribution of a synthetic Co-Åkermanite, Ca₂CoSi₂O₇, by using X-ray anomalous dispersion effect around Co K absorption edge. It is expected to inform us the incommensurate and super structure of the material, and local structure around Co atoms. The software for the procedure of the Weissenberg photograph has not been completely provided in DIP-320HL version of the control system of at the beam line. We therefore reconstruct a new software system to proceed the obtained Weissenberg photographs on IP, and to treat the intensity data in the computer system. at the points where the higher harmonics and superlattice diffractions are, and finally try to solve the modulated structure in detail. In this report, we present the results of the intensity measurements, and discuss the possibility of the improvement of the structure.

Experimental

The X-ray diffraction measurements of Weissenberg photograph were made on BL-1B beam line for Ca₂CoSi₂O₇ single crystal with the size in about 200 µm diameter. The specimen crystal was orientated for the 0 layer measurements of a*c* plane, then Weissenberg photographs were collected in the rotation axis of ω from -90 to 180 degree. Owing to the mechanical limitation of the translation moving of IP, a scan of the Weissenberg motion is made for each 3 degrees, and therefore the total numbers of the photographs is ninety. The photograph data were treated by the present software program named XVGW. The program has tree main functions: to combine the number of the Weissenberg photographs, to write out the photograph data on the memory of the system computer in Asccii code, to transform the combined Weissenberg photograph into the normal X*Y*Z* system in reciprocal space.

Results

An example of Weissenberg Photograph combined with ninety partial photographs is shown in Fig.1.



Fig.1 Weissenberg Photograph of Ca₂CoSi₂O₇. Ninety partial photographs are combined By XVGW program.



reciprocal plane.

The Wiessenberg photograph shown in Fig.1 is transformed to intensity distribution in reciprocal space, and the result is shown in Fig.2. The system is expected to be useful for quick survey of intensity distribution in reciprocal space, and thus effective for the intensity measurements such as a use of X-ray anomalous dispersion effects on the various diffractions.

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