10A/2005G161

X-ray diffuse scattering from protein crystals caused by the lattice defects

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Introduction

High resolution X-ray protein crystallography needs a single crystal of high quality.
The quality has been often described with a mosaicity. However, the intrinsic nature of the quality of a protein crystal has not yet been understood well. Phenomenologically speaking, a crystal of poor quality causes the decrease of the Bragg reflection intensity and does not give higher order Bragg reflections. It has been developed to estimate the quality of proteins by measuring the B-factor.[1] The B-factor consists of static and dynamic components and the quality of protein crystals may correspond to the orientation disorder of molecules in the crystal. The purpose of the study is to understand the relation between the molecular orientation disorder and the lattice defects by analyzing X-ray diffuse scattering.

Experiment

X-ray scattering intensity is described by eq.(1),

$$<I> = J_1 + J_2$$

$$J_1 = I_e |G|^2 |<F>|^2$$

$$J_2 = I_e \sum_{nn'}^{N} \exp\{2\pi i[\vec{K}\cdot\vec{R}_n - \vec{R}_{n'}]\} <(F_n - <F>)(F_{n'} - <F>)^*> \quad \cdots(1)$$

where J1 and J2 are Bragg reflection and diffuse scattering terns, respectively.
The J2 term has been extracted from the rocking curve profile of the Bragg reflection. The sample is a cubic insulin crystal which has given a medium resolution data set (2.2 Å) and the B-factor is 27.4 $Å^2$. The crystal size is about 0.3mm·0.3mm·0.3mm in length.We have used a 4-circle diffractometer installed at BL10A in Photon Factory in KEK. We have measured several rocking curves of Bragg reflections of [100], [110] and [111] series at the ambient temperature. The J2 term has been extracted by fitting two Gaussians on the experimental Data. Consequently, we have succeeded in observing the diffuse scattering at the foot of these Bragg reflections as shown in Fig.1. The diffuse scattering intensities of [100], [110] and [111] series were obtained by integrating the fitted Gaussians, and they are normalized by the corresponding Bragg reflections as shown in Fig.2. The ratio of the diffuse scattering intensity to the Bragg reflection is more or less 0.1, and there have not striking differences among [100], [110] and [111] series. In order to confirm the origin of these diffuse scatterings, we have a plan to explore the similar measurement by using the crystals of different qualities.

Reference

[1] S.Arai, T.Chatake, N.Suzuki, H.Mizuno and N.Niimura: Acta Cryst. D60, 1032-1039 (2004)

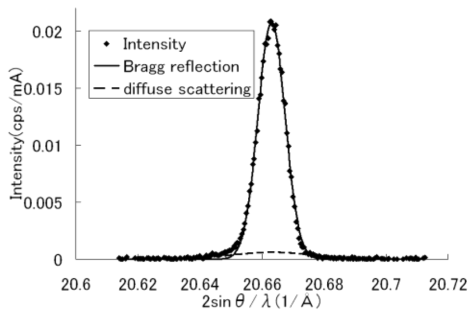

Fig.1 The observed rocking curve profile and the fitting of data Gaussian

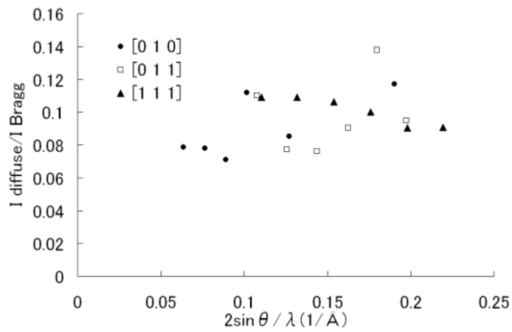

Fig.2 The integrated intensity of diffuse scattering normalized by the corresponding Bragg reflections vs 2sinθ/λ