Wide-band parallel synchrotron radiation beam and its application to the study of crystal structure

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This doctoral thesis describes development of the technique for obtaining wide-band parallel X-ray beam on a synchrotron radiation source and its application to derivation of structural information on solid materials.

X-ray diffraction method is the most powerful method to determine three- dimensional atomic arrangements in crystals, in which position and integrated intensity of Bragg reflections are measured in general using monochromatic X-ray beam. In this thesis it is shown that structural information can also be derived from the intensity profile of Bragg reflections. When diffraction measurements are made with X-ray beam of an energy close to the absorption edge of atoms in a crystal, characteristic structure appears in the intensity profile in which information on the phase of the crystal structure factor and the absolute configuration of an enantiomer is contained.

As the most efficient method of recording the intensity profile of Bragg reflections, use of the wide-band parallel X-ray beam is proposed with two methods for producing such a beam from synchrotron radiation source at Ritsumeikan University.

The intensity profile of one hundred Bragg reflections of a ferrocene derivative MPAF-5 were recorded and the phases of the crystal structure factors were successfully determined. From the intensity profiles of 17 Friedel pairs of Bragg reflections of another ferrocene derivative HPF, absolute configuration of the HPF molecule was unambiguously determined.

The intensity profile method using the wide-band parallel X-ray beam is shown to be a new, powerful, widely applicable method of structural study.