14-Diffraction Physics and Optics


X-ray crystallography of macromolecules is a most powerful technique to determine their three-dimensional structure. However, the technique has been limited to crystal samples of about 0.1mm, even by using synchrotron radiation. The synchrotron radiation from an undulator installed in the Spring-8, which is a third-generation synchrotron radiation facility in Japan now under construction, is characterized by a high-energy and a low-emittance. The character of high-energy is effective to eliminate the radiation damage to the crystal samples of macromolecules and the character of low-emittance is useful to obtain a small focal point. Therefore, the high-energy X-rays emitted from the undulator will open the macromolecular structure analysis to samples smaller than 0.1mm. However, a problem is that the reflectivity of total reflection mirrors, a conventional focusing element of X-rays, drops suddenly in the energy region over 20 keV. On the contrary, the reflectivity of perfect crystals such as silicon is maintained at one even for high-energy X-rays. Our purpose is to realize macromolecular crystallography with small sample crystals at the Spring-8 by developing a double-focusing perfect crystal monochromator which is bent in the horizontal and vertical directions simultaneously. We made a preanneal beryllium of silicon wafer, the thickness of which was 0.5mm. The border has two mechanisms for spreading spaces between four legs of a table-like copper block in the horizontal and vertical directions independently. The silicon wafer was glued tightly on the surface of the copper block. By using them, the required curvature radii in horizontal (about one meter) and vertical (several hundred meters) directions were achieved simultaneously with an energy resolution below 10^{-4} without any damage to the silicon wafer. The confirmation of its focusing character is now under progress.

The quasi-wave plate was placed between the curved crystal and the sample and its diffracting planes adjusted to make an angle ψ with the horizontal plane equal to 45° + a few degrees. In order to have a non-dispersive setup between the curved crystal and the phase plate, the interplanar distance of both reflections have to fulfill an exact relation where the angle ψ is a parameter. A nondispersive setup could thus be obtained with a silicon 311 reflection for the curved crystal; a 220 reflection of a diamond phase plate and an angle ψ equal to about 44°. Thanks to its low absorption coefficient, the diamond plate could be chosen thick enough to be adjusted rather far from the Bragg reflection (121 precise) in order not to be too sensitive to the divergence of each monochromatic beam (of the order of 1 minute) induced by the size of the source which is rather broad at LURE (2.35 σω = 63 mm, 2.35 σω = 36 mm).

The quasi-wave plate efficiency has been checked by measuring the Magnetic Circular X-ray Dichroism spectra (MCXD) of GdF2 and GdCu2 near the Gd L3 absorption edge using the linearly polarized beam in the orbit plane. The MCXD spectra were taken with the beam obtained classically using right-handed elliptically polarized photons selected by an horizontal slit adjusted below the orbit plane. It will be shown that the results are very similar. The polarization rate can then be evaluated to about 80%. The efficiency of the phase plate should be still higher for a smaller source and especially for the undulator assigned for beam line 6B at ESRF (Grenoble-France), where an energy dispersive absorption spectrometer will be available.

PS-14.01.15 COHERENT INELASTIC MOSSBAUER SCATTERING OF SYNCHROTRON RADIATION IN PERFECT CRYSTALS. By V. A. Belyakov, Surface and Vacuum Research Centre, 177334 Moscow, Russia

Coherent inelastic Mössbauer scattering (CIMS) of synchrotron radiation (SR) in perfect crystals containing nuclei of Mössbauer isotope is theoretically investigated. The equations describing the angular distribution of CIMS are presented in the form:

\[ \langle \text{rot} E_\omega \rangle = \langle \omega / c \rangle \langle \text{ rot} E_\omega \rangle = \langle 2 \rangle \langle E_\omega \rangle \]

where \( E_\omega \) and \( \omega \) are the electric field of CIMS and its frequency, \( \langle \rangle \) is the X-ray dielectric tensor of the crystal for zero abundance of Mössbauer isotope. \( E_\omega \) is the field at Mössbauer frequency experiencing elastic nuclear resonance scattering in the crystal and \( \langle \rangle \) is the "inelastic susceptibility" of the crystal determined by the structure and dynamical properties of the crystal and describing the change of the resonant photon frequency due to nuclear scattering accompanied by absorption or creation of a phonon in the crystal. The case of Mössbauer diffraction of SR under the conditions of excitation of a purely nuclear magnetic or quadrupole reflection forbidden for X-ray scattering (V. A. Belyakov, Diffraction Optics of Complex Structured Periodic Media, Springer Verlag, New York, 1992) is investigated in detail. In the limit of a thin crystal eq. (1) describes the kinematical results (V. A. Belyakov and Yu. M. Aivazian, NIM, A189, A282, 658-631) and, in particular, the results related to the CIMS angular distribution which is independent on the wave vector of a photon accompanying the inelastic scattering. So the directions of CIMS coincide with the directions of primary and diffracted beams in elastic Mössbauer scattering. The expres-