14-Diffraction Physics and Optics

PS-14.01.13 DEVELOPMENT OF A DOUBLE-FOCUSING MONOCHROMATOR FOR MACROMOLECULAR CRYSTALLOGRAPHY WITH SMALL SAMPLE CRYSTALS AT THE SPRING-8. N. Kamiya*, H. Iwasaki, T. Uruga, M. Yamamoto and T. Ueki, The Institute of Physical and Chemical Research (RIKEN), Hirosawa 2-1, Wako, Saitama, Japan 351-01.

X-ray crystallography of macromolecules is a most powerful technique to determine their three-dimensional structure. However, the technique has now been limited to crystal samples of about 0.1mm, even by using synchrotron radiation. The synchrotron radiation from an undulator installed in 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 that of low-emittance is useful to obtain a small focal point. Therefore, the high-energy X-rays emitted from the SPring-8 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 parfect crystals such as silicon is maintained as one even for high-energy X-rays. Our purpose is to realize macromolecular crystallography with small sample crystals at SPring-8 by developing a double-focusing perfect crystal monochromator which is bent in the horizontal and verical directions simultaneously.

We made a prototype bender of silicon wafer, the thickness of which was 0.5mm. The bender 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 a energy resolution below 10^{-3} without any damage to the silicon wafer. The confirmation of its focusing character is now under progress.

PS-14.01.14 ENERGY DISPERSIVE QUATER-WAVE PLATE FOR MAGNETIC CIRCULAR DICHROISM EXPERIMENTS IN THE X-RAY RANGE by C.Giles[1], C.Malgrange*[2], J.Goulon[1], F.de Bergevin[1,3], C.Vettier[1], E.Dartyge[4], A.Fontaine[4], C.Giorgetti[4], S.Pizzini[4].

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It is well known that linearly polarized photons can be transformed into circularly polarized ones by use of a quater-wave plate whose neutral lines make an angle of 45° with the polarization vector. For X-rays, such plates are obtained with perfect crystals set at or near a Bragg reflection. The neutral lines are then respectively perpendicular and parallel to the diffraction planes.

In the experiment described here, the beam transmitted by a crystal adjusted in Bragg geometry near the Bragg angle but outside the diffraction profile has been used as initially suggested by Dmitrienko and Belyakov (Sov.Techn.Phys.Lett., 1980, 6, 621-622) and successfully tested by Hirano et al. (Jpn.J.Appl.Phys., 1991, 30, L407-410) with a monochromatic and very well collimated beam.

Here, the phase plate has been designed to be incorporated in an energy dispersive X-ray absorption spectrometer and particularly at the DCI station at LURE (Orsay-France) where the quater-wave plate has been tested. In such a setup, a curved crystal diffracts in the horizontal plane a *divergent* and *polychromatic* beam and focuses it at a point where the sample is placed. After the sample, the beam diverges and the wavelengths are analyzed separately by an array of diodes.

The quater-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 then 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 (125 arcsec) 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 σ_x = 6.3 mm, 2.35 σ_y = 3.6 mm).

The quater-wave plate efficiency has been checked by measuring the Magnetic Circular X-ray Dichroism spectra (MCXD) of $GdFe_2$ and $GdCo_2$ near the Gd L_{III} absorption edge using the linearly polarized beam in the orbit plane. The MCXD spectra have been compared to that 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 designed for beam line #8 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:

$$\mathrm{rotrot}E_{in} - (\omega/c)^2\varepsilon(r)E_{in} = \chi(r)E_{el}, (1)$$

where E_{in} and ω are the electric field of CIMS wave and its frequency, $\varepsilon(r)$ is the X-ray dielectric tensor of the crystal for zero abundance of Mössbauer isotope, E_{el} is the field at Mössbauer frequency experiencing elastic nuclear resonance scattering in the crystal and $\chi(r)$ 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 details. In the limit of a thin crystal eq. (1) describes the kinematical results (V. A. Belyakov and Yu. M. Aivazian, NIM, 1989, A282, 628-631) 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-

