Rapid & Sensitive XAFS Using Tunable X-Ray Undulator

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1. Ray Tracing

As an optics for a standard undulator (32V) beamline XU10, a double-crystal monochromator with a rotated-inclined geometry [1] is considered. Reflectivities for a double-crystal (+,-) configuration and a four-crystal (+,-,-,+) configuration were calculated by a dynamical theory for the Si(111) and Si(220) reflections. Inspection of DuMond diagrams showed that the angular divergence for the first pair of four-crystal setup is almost equal to that of the last pair. For a rotated-inclined double crystal where ***k*** and ***n*** represent vectors for the incident beam and surface normal, the axis of crystal rotation ϕ around the vertical axis z is given by the following equation.

$$\phi=\sin^{-1}\{(\cos\alpha-\sin\theta_B\sin\psi)/\cos\theta_B\cos\psi\} \qquad (1)$$

where α is the angle between ***k*** and ***n*** and ψ is the tilt angle of the crystal surface which is assumed to be 10°. ϕ is calculated to be 1.529° ($\theta_B=14.31^\circ$) and 0.347. ($\theta_B=7.73^\circ$) for Si(111) and Si(220) reflections, respectively.

For a grazing-incidence angle of 1°, the power density on the first crystal surface ~ 5 W/mm^2 is reduced to 1/57.3. The FWHM values for rocking curves are 14.9 arcsec at 8 keV for Si(111) and 2.3 arcsec at 24 keV Si(220). Because of asymmetric reflection of a rotated-inclined geometry, calculated FWHM values are greater than those of a conventional symmetric diffraction: the magnitude of asymmetry factor b is 0.26 and 0.60 for the Si(111) and Si(220) reflections, respectively. The calculated energy resolution $\Delta E/E$ given as the convolution of rocking curve width and an angular divergence multiplied by $\cot\theta_B$ is 2.6 x 10^{-4} at 8 keV and 7.6 x 10^{-5} at 24 keV, respectively. In Fig.1 , the results of ray tracing are shown for various points from the source.

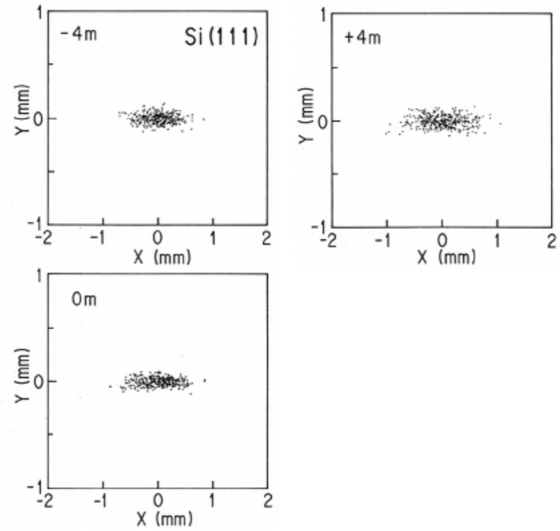

Fig.1 Spot profile of undulator radiation around the sample position.

2. Detector

In the experimental hutch of XU10, a 100-element "monolithic" Ge detector array is to be installed together with the goniometer for the polarized fluorescence XAFS . The arrangements of Ge elements are illustrated in Fig. 2, together with a 19-element Ge detector based on a conventional technique of assembling independent element with a close packing arrangement [2] . In the latter arrangement, the packing ratio is 57% which incresed from the previous standard 13-element detector (38%) [3].

In a monolithic approach, the dead region between the two elements is only 10 micron.

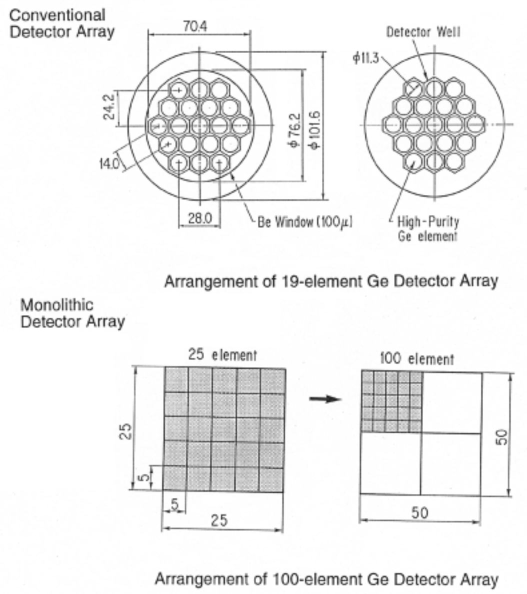

Fig.2 Arrangements of detector elements for 19-elment and 100-element Ge detectors.

In this design, each element is 10 mm thick and has an effective area of 5 mm x 5 mm. A typical energy resolution is 190 eV at 5.9 keV at a medium count rate. We estimate the energy resolution at a high count rate (3 x 10^5 cps) to be about 240 eV using a 0.5 msec time constant.

Each detector element is equipped with PSC941 preamplifier (Penta FET). In total, 3 x 10^7 cps is expected. For energy analysis and counting, a digital signal processor (DXP, X-ray Instrum. Assoc.) is used. Each module has 4 input channels for which an energy analysis based on a digital signal processor is available. In total, DXP 25 modules are controlled by a work station running on linux 2.1 via CAMAC interface. The data acquisition software is a modified version of the SCAN developed by Oyanagi et al. [4] which has been recently revised to be compatible with UNIX operating system in C.

In Fig. 3, the electronics and control system of the 100-element Ge detector is shown.

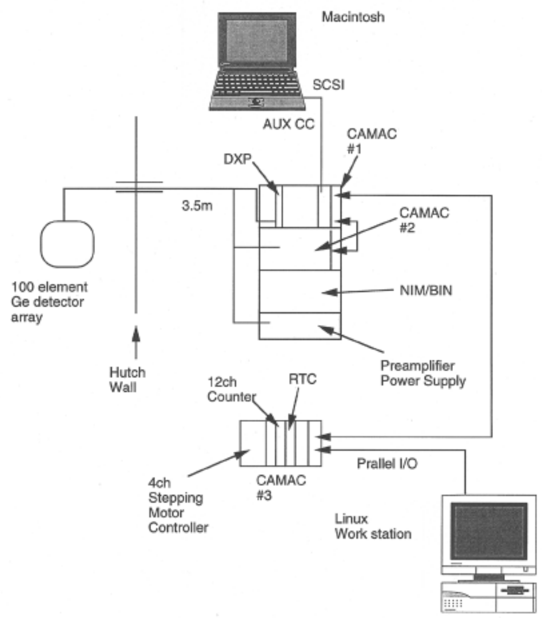

Fig.3 Electronics for 100-element Ge detector and control system.

3. Experimental Setup

In the experimental hutch, the 3-axis goniometer is installed. A He closed cycle refrigerator can be either vertically or horizontally arranged, for the purpose of two different polarization geometries . The intermediate angle of incidence is aloso available. In addition to the omega rotation (sample rotation) and c axis for varying the angle of incidence, we added 2q motion for the transmitted and/or reflected beam intensity monitor. This allows us to measure also the X-ray standing wave using a fluorescence detector for XAFS experiments . An ionization beam monitor is attatched to the 2q arm and rotate around a horizontal axis.

In Fig.4, apparatuses for the future experiments are also shown. Using a high brilliance X-ray beam available from an undulator, we plan a "pump and probe" experiment. The first experiment for photo-induced structural change in amorphous selenium [5] is promising. *In-situ* monitoring of the local structure in amorphous selenium under illumination at low temperature shows the bond alternation associated with a photoexcitation. This suggests that the dominant process of photoexcitation of lone pair electrons is the formation of neutral three-fold coordinated defect pairs linking two adjacent spiral chains .

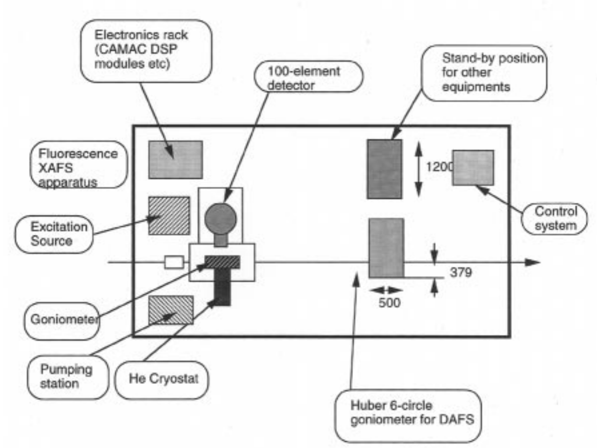

Fig.4 Plan view of the experimental hutch.

References

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