A NEW CAUCHOIS-TYPE COMPTON SCATTERING SPECTROMETER FOR HIGH-Z MATERIAL RESEARCH

The structure of the Fermi Surface (FS) is one of the defining properties of a metallic ground state, which is considered to be directly responsible for a number of scientifically interesting phenomena including magnetic ordering, compositional ordering, and superconducting. In a Compton scattering experiment, one measures the momentum density distribution,

$$J(p_z) = \iint n(\mathbf{p}) dp_x dp_y \ ,$$

where $n(\mathbf{p})$ is the ground state electron momentum density. The FS marks the boundary between occupied and unoccupied states in momentum space. Therefore, the Compton profile $J(p_z)$ contains fingerprints of FS breaks in the underlying 3-dimensional momentum density distribution $n(\mathbf{p})$. The FS can be directly mapped out by reconstructing the $n(\mathbf{p})$ through a few dozen $J(p_z)$'s measured along different crystallographic directions.

Until now, extension of this unique capability of the Compton scattering technique to the FS of high-Z materials (*e.g.* high-Tc superconductor, 4*f*, 5*f* heavy fermion systems) has been difficult because the incident X-ray energies available in current high-resolution spectrometers are too low to measure Compton profiles due to strong absorption of the samples. For the purpose of FS studies on high-Z materials, we have installed a new high-resolution Compton scattering spectrometer at beamline **BL08W**, operating with 115 keV incident X-ray energy, making it possible to obtain the Compton profiles of virtually all materials [1].

As shown in Fig. 1, the spectrometer consists of a Cauchois-type bent-crystal analyzer and a Ge solid-state detector (SSD1) as a position sensitive detector (PSD) with four 200 µm wide slits. Since the Ge-SSD is also an energy analyzer, it is very effective to discriminate the signal from the background noise. The SSD1 is mounted on a moving stage, and covers the position corresponding to the energy range from 70 to 90 keV for the incident X-ray energy of 115 keV and the scattering angle of 165 degrees. The distances between the sample and the bent-crystal analyzer, and between the bent-crystal analyzer and the detector are 500 mm and 3500 mm, respectively. The SSD2 simultaneously measures the Compton profile in order to monitor the intensity of the incident X-rays. Figure 2 shows the Cauchois-type bent-crystal analyzer assembly. The analyzer

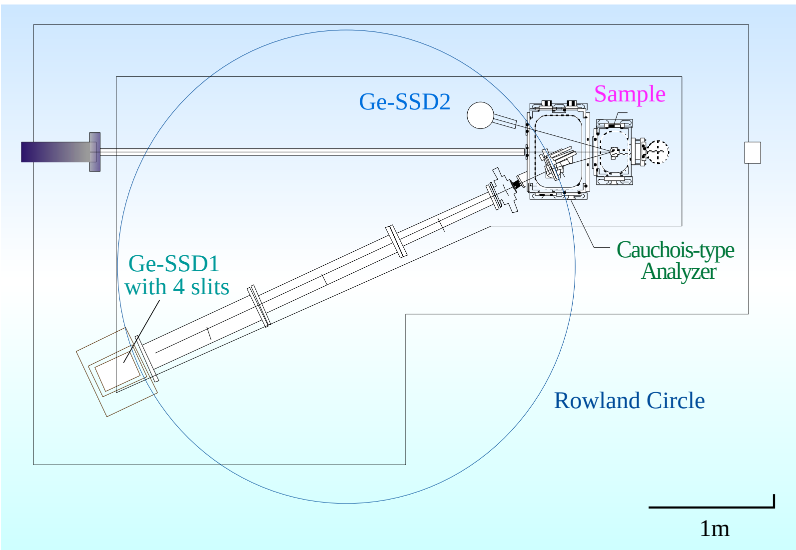
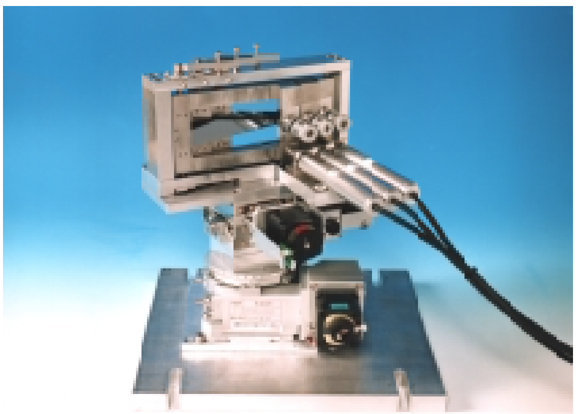


Fig. 1. Schematic setup of the Cauchois-type high-resolution Compton spectrometer.

assembly is made up of three separate triangle bent-crystals of Si 620 with 1 mm thickness, and is equipped with a Bragg-angle adjuster for each bent-crystal. This analyzer assembly system has obtained three times higher efficiency than a single bent-crystal. Without any detectable degradation of the shape and width of the Bi-Kα1 fluorescence line at 77 keV, an energy resolution of 100 eV in FWHM has been achieved. Consequently, an overall momentum resolution of 0.13 atomic units has been achieved, in which the incident X-ray energy width of 160 eV has been taken into account.

Compton profiles of Nb have been measured along the [100] and [110] directions in order to demonstrate the performance of the spectrometer. The raw profiles were corrected for the background noise, the energy-dependent efficiencies of the crystal analyzer and the Ge-SSD1, the absorption of the sample, the energy-dependent Compton scattering cross section and the Compton double scattering of the sample. The valence Compton profiles are shown in Fig. 3(a), together with those from LDA-FLAPW band theoretical calculations. The anisotropy of the profiles is shown in Fig. 3(b) as well. The theory and experiments show excellent agreement in the fine structures of the profiles and the anisotropy. The theory predicts that the first band in Nb is completely filled, and the second band has a closed hole surface centered at the point Γ. The third band has closed hole pockets at the points N and a multiply connected jungle-gym hole surface consisting of interconnecting arms along <100> directions. The present experiments have succeeded in identifying the complex FS signatures of Nb. The fine structures found in the valence Compton profiles are considered to originate from the shape of the closed hole pockets and the jungle-gym hole surface in the third band.

To carry out the direct FS mapping by the reconstruction method, a 10-fold increase in the data-acquisition efficiency is strongly required. Replacement of the present SSD1 by a PSD with the same energy resolution could aid in achieving the increase in efficiency. A μ-strip Ge PSD with an area of 100×40 mm^2 is currently under development and could be used to solve this problem.



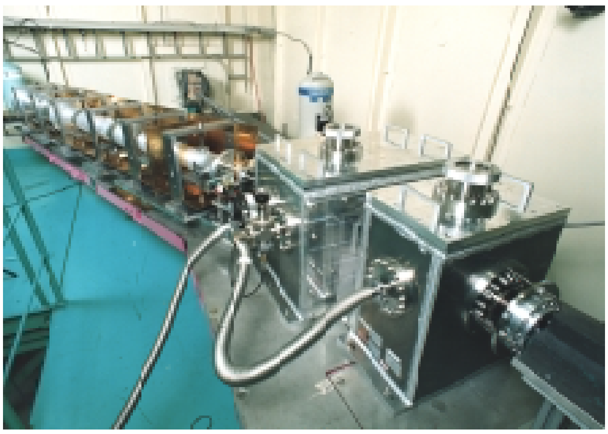


Fig. 2. Cauchois-type analyzer assembly, consisting of three separate triangle bent-crystals of Si 620 with 1 mm thickness.

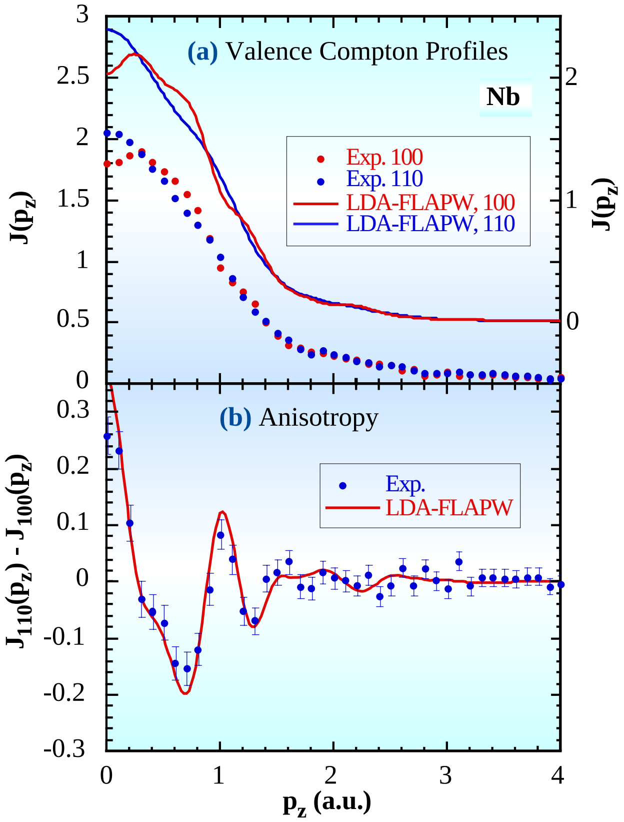


*Fig. 3. **(a)** Compton profiles of the valence electrons of Nb along the [100] and [110] directions. **(b)** Anisotropy between the [100] and [110] directions.*

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References

[1] Y. Sakurai, J. Synchrotron Rad. **5** (1998) 208.