

Spin moment determination of ferro- or ferrimagnetic materials using magnetic Compton scattering

Yoshiharu Sakurai

Japan Synchrotron Radiation Research Institute

1. Introduction to Compton scattering and magnetic Compton scattering

(1) Compton Scattering [1]

Most students remember learning the Compton effect, i.e. the effect of Compton scattering, from an introductory textbook on quantum ideas. The Compton effect, the increase in the wavelength, i.e. the decrease in the energy, of X-rays and gamma-rays on being scattered by material objects, clearly demonstrates that X-rays and gamma-rays have a particle nature and these particles, the photons, behave like materials particles in collisions with electrons in material objects. Considering a collision between a photon and an electron, conservation laws for energy and momentum lead to a simple result for the energy shift (ΔE) of a photon by Compton scattering,

$$\Delta E = \frac{\hbar^2 \mathbf{q}^2}{2m} + \frac{\hbar \mathbf{q} \cdot \mathbf{p}}{m}, \quad (1)$$

where \mathbf{p} is the electron momentum before scattering, \mathbf{q} the scattering vector, m the electron mass. The first term corresponds to the fixed shift in energy only depending on the scattering geometry, and the second term is a Doppler shift that depends on the component of the electron momentum \mathbf{p} along the scattering vector \mathbf{q} . Therefore, the Compton-scattered X-ray line is broadened by moving electrons (see Fig.1). Under an impulse approximation, the line shape is in proportion to the so-called Compton profile, $J(p_z)$,

$$J(p_z) = \iint n(p_x, p_y, p_z) dp_x dp_y, \quad (2)$$

where $n(p_x, p_y, p_z)$ is the probability distribution of the electron momenta in material object and the z direction is taken along the scattering vector \mathbf{q} . The Compton profile can be normalized to the total number of electrons N in the material object,

$$\int J(p_z) dp_z = N. \quad (3)$$

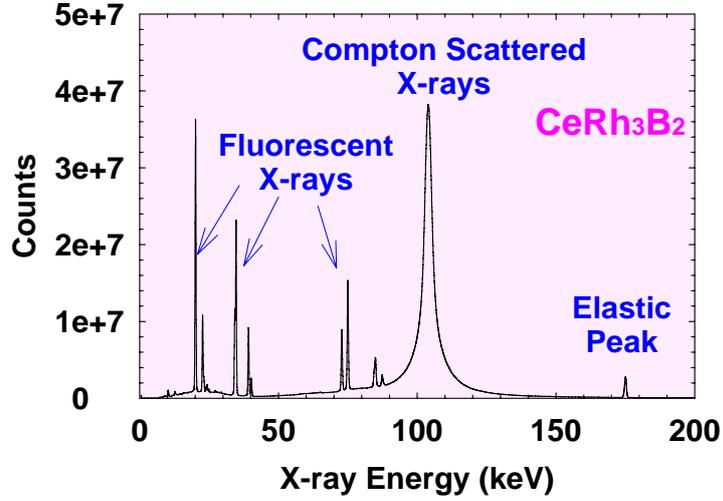


Fig.1: X-ray energy spectrum from CeRh_3B_2 measured by a Ge-SSD with a scattering angle of 168 degrees. The incident X-ray energy is 175 keV at Elastic Peak and the Compton scattered X-ray line at 105 keV is broadened by Doppler-shift in collision between the photons and moving electrons.

(2) Magnetic Compton Scattering [2]

When the X-rays are circularly polarized and the material object is a ferro- or ferromagnetic material, the Compton-scattered X-ray line shape is proportional to the scattering cross section,

$$\frac{d^2\sigma}{d\Omega d\omega} = C \cdot J(p_z) + C_{mag} \cdot P_C \cdot \mathbf{S} \cdot (\mathbf{k} \cos \theta + \mathbf{k}') J_{mag}(p_z), \quad (4)$$

where P_C is the degree of circular polarization of X-rays, \mathbf{S} the spin direction, \mathbf{k} (\mathbf{k}') the wavevector of incident (scattered) x-rays, θ the scattering angle. C and C_{mag} are constants. The first term corresponds to the eq.(2) and the second term is the magnetic term which includes the magnetic Compton profile $J_{mag}(p_z)$,

$$J_{mag}(p_z) = \iint [n_{up}(\mathbf{p}) - n_{down}(\mathbf{p})] dp_x dp_y, \quad (5)$$

$$\mathbf{p} = (p_x, p_y, p_z)$$

where $n_{up}(\mathbf{p})$ and $n_{down}(\mathbf{p})$ are the probability distribution of the electron momenta for up-spin electrons and down-spin electrons in a ferromagnetic material. The magnetic Compton profile can be normalized to the difference in the numbers of up-spin and down-spin electrons, i.e spin moment μ_{spin} (μ_B) for $g=2$,

$$\begin{aligned}
\int J_{mag}(p_z) dp_z &= \iiint n_{up}(\mathbf{p}) dp_x dp_y dp_z - \iiint n_{down}(\mathbf{p}) dp_x dp_y dp_z \\
&= N_{up} - N_{down} \\
&= \mu_{spin} (\mu_B)
\end{aligned} \quad (6)$$

The second term in eq.(4) can be isolated by changing the degree of circular polarization of incident X-rays P_c or changing the spin direction \mathbf{S} in a ferromagnet. Usually, the spin direction is changed by external magnetic field for isolating the magnetic term. Figure 2 shows spectra of Compton scattered X-rays from a polycrystalline Fe with different spin directions (Positive and Negative), together with the difference between the Positive and Negative spectra (Difference), i.e. magnetic Compton profile.

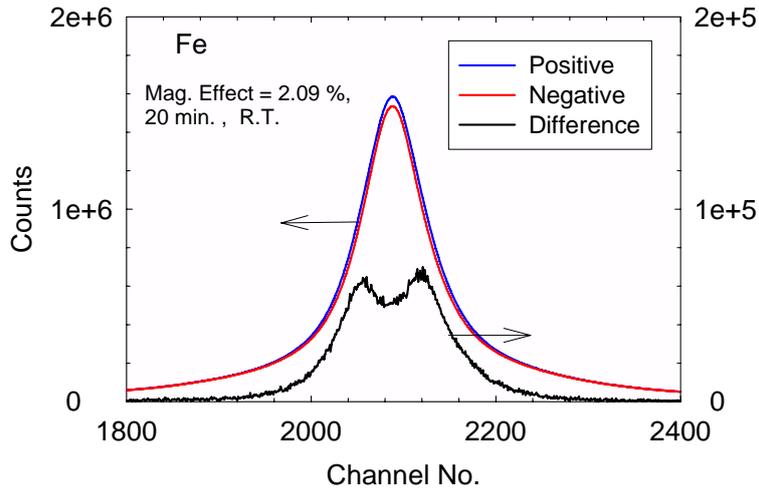


Fig.2: Spectra of Compton scattered X-rays from Fe with positive and negative spin directions, together with the difference spectrum (magnetic Compton profile) between them.

2. Spin moment determination [3]

In order to determine the absolute spin moment in a sample, the magnetic effect R is defined by the following equation,

$$R = \frac{I^+ - I^-}{I^+ + I^-}, \quad (7)$$

where I^+ and I^- are the integrated intensity of Compton scattered X-ray spectra measured when the spin direction, i.e. the direction of external magnetic field, is parallel

(+) and anti-parallel (-) to the scattering vector. On the other, using eqs.(3), (4) and (6),

$$\begin{aligned}
 I^+ - I^- &= 2C_{mag} \cdot P_C \cdot \mathbf{S} \cdot (\mathbf{k} \cos \theta + \mathbf{k}') \int J_{mag}(p_z) dp_z \\
 &= 2C_{mag} \cdot P_C \cdot \mathbf{S} \cdot (\mathbf{k} \cos \theta + \mathbf{k}') \cdot \mu_{spin}, \\
 I^+ + I^- &= 2C \int J(p_z) dp_z = 2C \cdot N,
 \end{aligned} \tag{8}$$

and thus the magnetic effect R is given by,

$$R = A \left(\frac{\mu_{spin}}{N} \right), \tag{9}$$

where μ_{spin} is the spin moment and N the total number of electrons, again. Once the coefficient A is given, the spin moment can be determined from the experimentally determined magnetic effect R through eq.(9) since the total number of electrons N is known. The coefficient A is usually determined by measurement on a well-characterized ferromagnet, such as Fe, in which its spin moment is already known. Figure 3 shows the relationship between the experimentally obtained R and μ_{spin}/N for Fe, Co, Ni, LSMO and SRO in which their spin moments are determined by other methods.

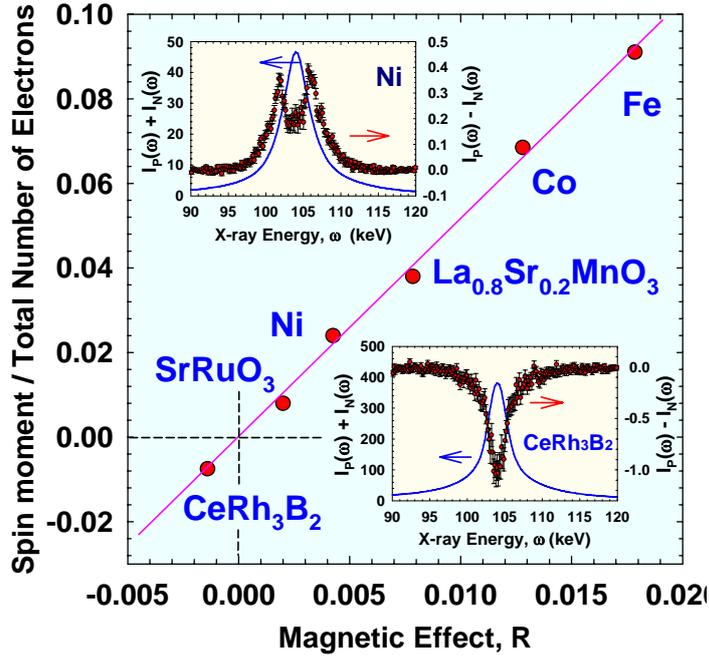


Fig.3: Relationship between the magnetic effect R and μ_{spin}/N for Fe, Co, Ni, LSMO and SRO in which their spin moments are determined by other methods.

3. Experimental Setup: Magnetic Compton Scattering Spectrometer

Figure 4 show the magnetic Compton scattering spectrometer at the BL08Wbeamline. The spectrometer consists of a 3T-superconducting magnet, a sample cryo-cooler and a 10-element Ge SSD. The superconducting magnet can reverse the magnetic field in few seconds between -2.5 T and +2.5T and the cryo-cooler can hold the sample at a temperature between 5 K and R.T. The incident X-rays are elliptically polarized and their energy is 175 keV. Compton scattered X-rays from a sample are detected by the 10-element Ge SSD at a scattering angle of 178 degrees.

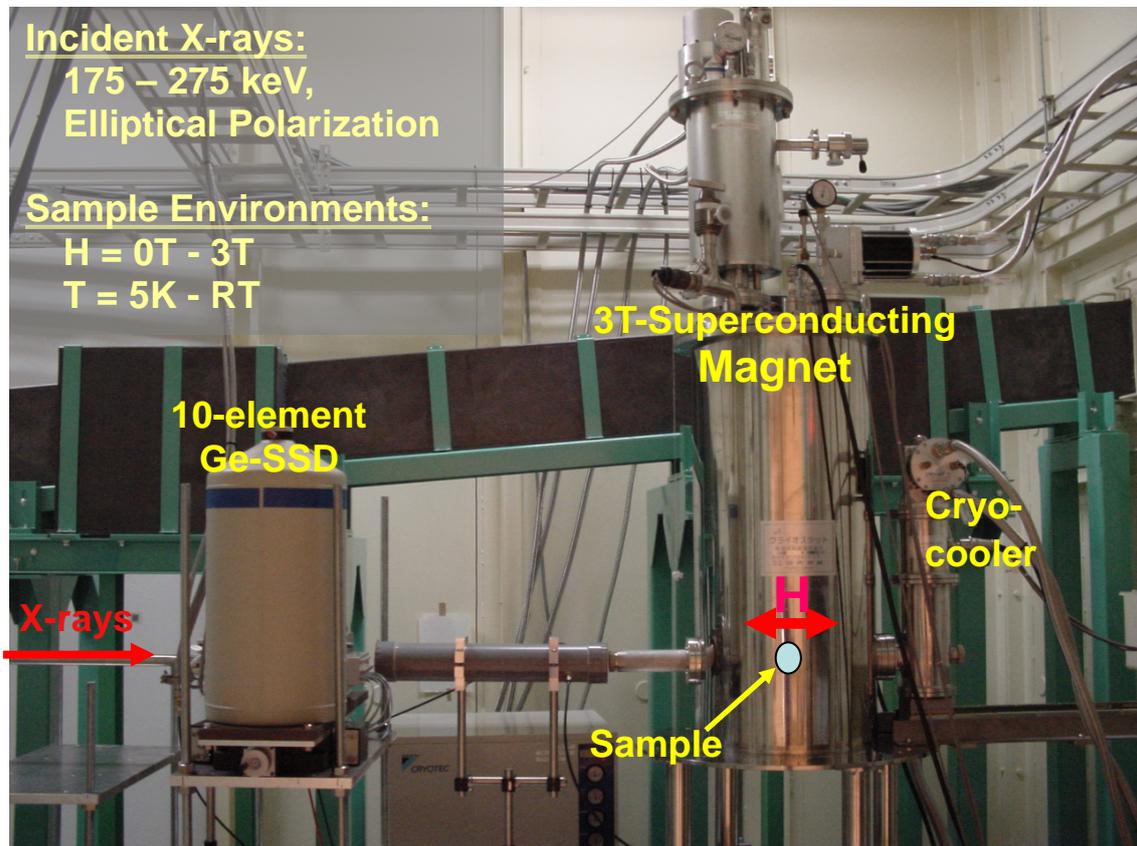


Fig.4: Magnetic Compton scattering spectrometer at BL08W

4. Practice

In the beamline practice (BL08W), we measure three ferromagnetic samples, Fe, Ni and CeRh₃B₂.

Firstly, we measure polycrystalline samples of Fe and Ni at room temperature. The aim of this experiment is to see that the magnitude of magnetic effect depends on the value of spin moment. The spin moments on Fe and Ni are 2.083 μ_B and 0.512 μ_B from other measurements.

Secondly, we measure a single crystal of CeRh₃B₂ at 10 K. The aim is to see that the magnetic effect is negative due to the presence of significant orbital moment in this Ce compound [3].

5. References

- [1] see, *X-ray Compton Scattering*, eds M. J. Cooper et al., Oxford University Press 2004.
- [2] N. Sakai, *J. Appl. Crystallogr.* **29** (1996) 81.
- [3] Y. Sakurai, M. Itou, J. Tamura-Okada, S. Nanao, A. Thamizhavel, Y. Inada, A. Galatanu, E. Yamamoto and Y. Onuki, *J. Phys.: Condens. Matter* **15** (2003) S2183.