Fermi-surface mapping on Complex materials using the 90 keV- new Compton spectrometer

N. Hiraoka, T. Buslaps , V. Honkimäki and P. Suortti*
ESRF (ID15)

A new Compton spectrometer has been constructed at ID15B, ESRF. This spectrometer provides a higher count rate with a better momentum resolution using 90-keV high energy X-rays, compared with the 60- and 30-keV ones, currently operating. We show that it is possible to routinely carry out a 2D Fermi surface reconstruction experiment on complex materials, which include heavy elements, in a reasonable beam time (- one week).

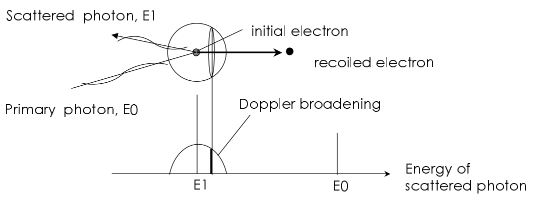
Why do we study Fermi surface ?

- The many of transport properties of solids, e.g. resistivity (including superconductivity), thermal conductivity, are understood based on behaviours of conduction electrons. In momentum space, the conduction electrons can be described by characteristic structures, so-called **Fermi surface(s)**, whereas in real space they are represented by extended wavefunction. Fermi surface is defined as the boundary between occupied and unoccupied states in momentum space.

How do we investigate Fermi surface(s) ?

- Compton profile measurement, reconstruction and LCW folding

- Compton scattering energy spectrum would show a single line, which is uniquely determined by the scattering geometry (energy-momentum conservation), for an ideally stationary electron. An actual spectrum is broadened because of the **Doppler shift, resulting from the primary momentum** of the electron contained in a sample. **Compton profile experiments** investigate the electron momentum distribution by analysing this Doppler broadening.



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

$$p_Z = mc \cdot (E_1 - E_0 + E_0 E_1 (1-\cos\theta)\cdot m^{-1}c^{-2})\cdot(E_0{}^2 + E_1{}^2 - 2E_0 E_1 \cos\theta)^{-1/2}$$

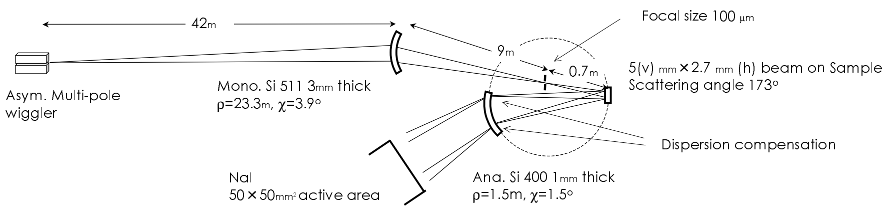
- The Doppler broadening provides information only about the momentum along the scattering axis (p_z direction) , whereas it integrates the momentum density along the other axes. The integral(s) can be solved by a **reconstruction technique** with CP's measured on several directions. Finally, Fermi surface signals are enhanced by folding the momentum density into a 1st Brillouin with respect to reciprocal lattice vectors **G**'s, so-called **Locks-Crips-West (LCW) folding**.

However, a reconstruction experiment is rather time-consuming because data have to be taken with high statistics and a good resolution for all directional profiles in order to extract weak and fine Fermi surface signals. It is even more serious for complex materials, comprising many electrons irrelevant to the Fermi surface.

How do we get good data (in limited beam time) ?

- 90-keV new Compton spectrometer

- The idea of the spectrometer is based on the combination of two bent Laue crystals. The bent Laue monochromator leads to a better focusing (for resolution) and an optimisation of a band width (for flux) yet a large energy gradient (~2 keV at 90 keV). The analyser operates with so-called Dispersion compensation geometry to compensate the large energy gradient from the monochromator. Since the Compton shift (E_o-E_1) is independent of the primary energy, the analyser reflects various energy but same p_z X-rays. [P. Suortti et al. NIM **A467** 1541 (2001)]



Count Rate at Compton peak	1200cps [/ 40 mA] (0.5 mm thick Al) 1000cps [/ 200mA](2 mm thick (Ba,K)Bio$_3$) 1500cps [/ 200mA](0.5 mm thick Mo$_4$O$_{11}$)
Resolution	0.08 au, i.e. ~1/10G (Al : optimum)* 0.12 au, i.e. ~1/6G ((Ba,K)Bio$_3$) 0.16 au, i.e. ~1/4Gc (Mo$_4$O$_{11}$))
Beam size at sample position	5 mm by 2.7 mm (full beam) 5 mm by 1.5 mm ((Ba,K)Bio$_3$) 3 mm by 0.8 mm (Mo$_4$O$_{11}$)

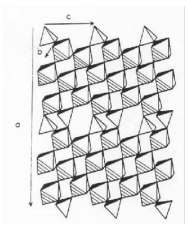
* Achieved best resolution is 0.06 au with 50 % lose of count rate

Results

η-Mo_4O_{11}

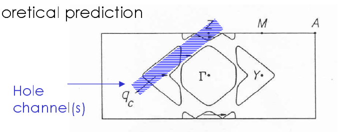
- Typical low-dimentional (2D) material, an anomaly of resistivity at 109K due to the charge density wave (CDW) . From the theoretical point of view, it is believed that the CDW originates from an instability in the Fermi surface geometry. The theoretical Fermi surface needs to be examined by experiments.

Orthorhombic crystal structure
Each O's octa(tetra)-hedron comprises one Mo atom



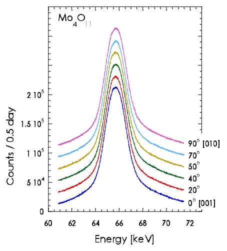
C. Schlenker et al. Phil. Magazine **B52** 646 (1985)

Theoretical prediction



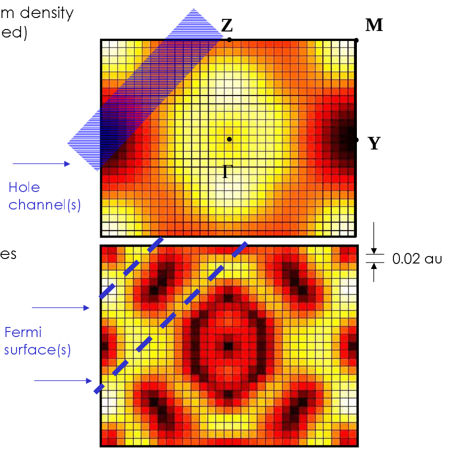
E. Canadell et al Inorg. Chem. 28 1466 (1989)

Raw profiles



Momentum density (LCW-folded)

Derivatives

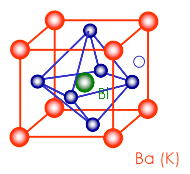


➡ **We have observed the important feature of the Fermi surfaces (for CDW), hole channels running from Y to Z, in the momentum density. It validates the adequacy of the theoretical Fermi surface.**

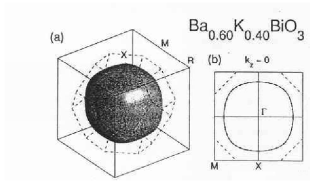
$Ba_{1-\delta}K_\delta BiO_3$

- 3 D-superconductor, metal-insulator transition at δ~0.3, accompanied with several structural transitions (cubic – orthorhombic - monoclinic) due to a CDW instability. Fermi surface is crucial information in understanding of these complicated phenomena.

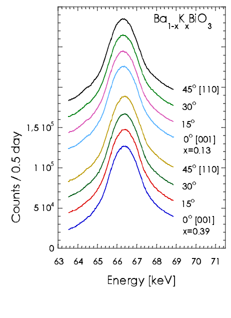
Perovskite-type (pseudo) cubic structure



Theoretical prediction of Fermi surface
S. Sahrakorpi et al. PRB **61** 7388 (2000)



Raw profiles

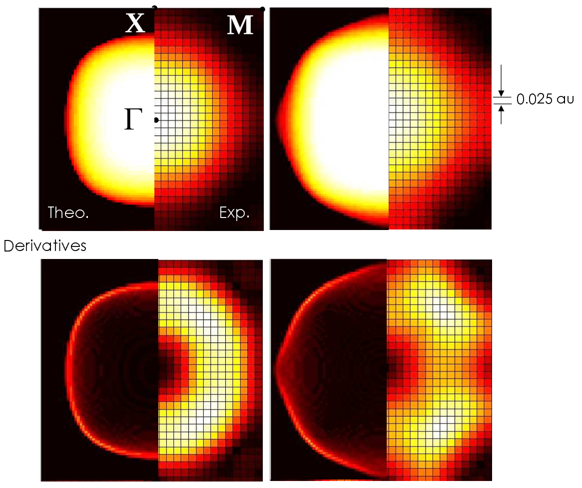


Momentum density (LCW-folded)

δ=0.39 (metal)

δ=0.13 (insulator-like)

Derivatives



➡ **The Fermi surface evolution, caused by K-doping, has clearly been detected in the momentum densities. The square-like shape of the experimental data at δ=0.13, not seen in the theory, seems to represent the modification of the Fermi surface by CDW. (Analysis still in progress)**

Acknowledgements

*initiated the project of the 90 keV Compton spectrometer construction (present affiliation : Univ. of Helsinki) .
The results on Mn_4O_{11} and $Ba_{1-\delta}K_\delta BiO_3$ were obtained under collaborations with Prof. Schlenker & Dr. Guyot (CNRS, Grenoble, France) and Prof. Uwe & Dr. Minami (Univ. of Tsukuba, Japan), respectively. We would also like to thank Dr. Tanaka (RIKEN, Japan) for providing the reconstruction program.