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# Three-dimensional electron momentum density in Si

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## Introduction

Compton profile measurements have been extensively used to study electronic structure of materials. Compton profile usually denoted as $J(p_z)$, $p_z$ being taken along the photon scattering vector, is electron momentum density $\rho(\mathbf{p})$ integrated over two momentum components $p_x$ and $p_y$. To explore electronic structure in greater detail, however, it is best to obtain $\rho(\mathbf{p})$ directly from experiment. For this purpose we have developed an (X-eX) spectrometer which can directly observe $\rho(\mathbf{p})$. The details of the spectrometer are described in the preceding report. In this report we present some of the results on electron momentum density in Si observed by this spectrometer.

## Preparation of thin foil of single crystal Si

The spectrometer measures the direction and energy of the recoiled electrons by a time of-flight method and the direction of Compton scattered photons in coincidence mode. Therefore, a sample should be thin enough for the recoiled electrons to come out without being additionally scattered in the sample. In the present experimental conditions the incident photons have an energy of 115.6 keV, the center of the energy spectrum of the recoiled electrons is 34.6 keV and that of the Compton scattered photons is 81.0 keV. We estimated the mean free path of an electron of 34.5 keV to be 43 nm using the total cross-section for elastic scattering given by the Wentzel model. Therefore, the thickness of the sample should be less than 100 nm. To prepare a 100 nm thick sample we utilize commercially available silicon-on insulator (SOI) wafers. A cross-section of the SOI is schematically shown in Fig. 1. We paste the 100 nm Si side to a sapphire plate by wax and mask the Si substrate side also with wax but leaving an unmasked area of about 5 mm in diameter, then chemically etch the Si substrate and $SiO_2$ layer. Finally we dissolve the wax to retrieve the 100 nm Si foil supported by the SOI wafer. In the following we present results obtained by using a single crystal foil whose plane normal is [100].

## Observed electron momentum density

Figure 2 shows the observed $\rho(\mathbf{p})$ on the (110) plane. In a region of ± 0.5 a.u. anisotropic momentum density with two-fold symmetry is clearly observed. Figure 3(a) shows the section along the [100] axis and 3(b) shows the section along the [111] axis. The full line represents theoretical results obtained by Kubo [1] using the FLAPW method. The theoretical curve is convoluted with the present experimental resolution. The experiment is normalized to the theory at p=0. Overall shape of the experimental momentum density is well reproduced by the theory. However, noticeable discrepancy between theory and experiment is found in the tail part where the experimental curve is higher than the theoretical curve. We speculate one of the causes of the discrepancy to be multiple scattering of the recoiled electrons in the sample.

## References

[1] Y. Kubo, private communication.

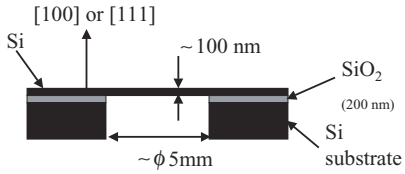


Fig. 1 Schematic drawing of a cross-section of a SOI wafer and a thin foil Si single crystal.

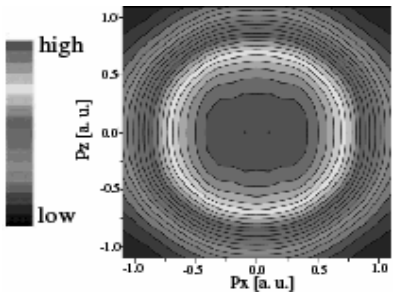


Fig. 2 Observed electron momentum density in Si on the (110) plane.$p_z$ is in the [001] direction and $p_x$ is in the [110] direction.

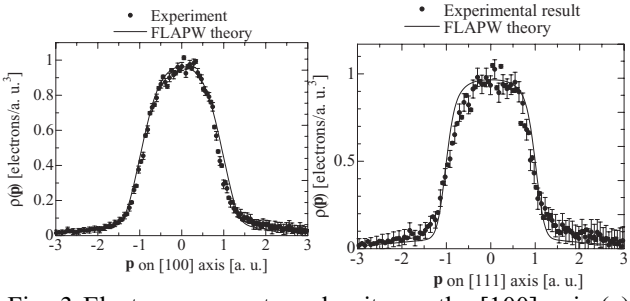


Fig. 3 Electron momentum density on the [100] axis (a) and on the [111] axis (b).