

Electron momentum density of hexagonal zinc studied by high-resolution Compton scattering

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Compton scattering is a powerful method for investigating the electronic structure of condensed matter. The spectrum of inelastically scattered monoenergetic photon beam in a target is related through the Doppler effect to the momentum density distribution $\rho(\mathbf{p})$, which is directly connected with the electron wave function in reciprocal space $\chi(\mathbf{p})$ and hence with the Fourier transform of the wave function in real space $\psi(\mathbf{r})$:

$$\rho(\mathbf{p}) = |\chi(\mathbf{p})|^2 = \left| \int \psi(\mathbf{r}) e^{i\mathbf{p}\cdot\mathbf{r}} d^3r \right|^2$$

Thus the Compton scattering technique is the most direct test of solid state theories, where electron wave functions are calculated from the first principles.

The final result of single Compton scattering experiment is the Compton profile (CP, $J(p_z)$), which is the one-dimensional projection (double integral) of the electron momentum density $\rho(\mathbf{p})$ onto the scattering vector direction (usually chosen as Z axis):

$$J(p_z) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho(\mathbf{p}) dp_x dp_y$$

Contribution to CP from core electrons is isotropic, but valence electrons contribution is modified by the crystal potential in solid. Therefore CPs differ when measured in different crystallographic directions set along the scattering vector. Subtraction of the profiles measured at two different directions removes all isotropic contributions to the profiles and forms the so-called difference profile. Difference profiles show the anisotropy of the electron momentum density. Small effects are then emphasized and sharp features near Fermi momentum begin to appear after subtraction.

Theoretical KKR calculations of Zn directional CPs were calculated by S. Kaprzyk and already presented in [1] and [2]. In this theory the electron wave functions outside the muffin-tin spheres are approximated by the combination of spherical harmonics. The Lam-Platzman correction for the correlated electron gas was also included. Medium resolution (0.42 a.u.) experimental CP anisotropies measured with the use of 662 keV radiation from ¹³⁷Cs isotope source at University of Białystok [1]

shows reasonably good agreement with theoretical KKR calculations except the low momentum region (up to 1 a.u.). High resolution (0.16 a.u.) anisotropies measured later with the use of 57 keV synchrotron radiation in ESRF [2] showed even worse agreement with KKR theory. This motivated us to measure the high resolution directional Compton profiles once more. The new high resolution (0.12 a.u.) experiment was performed in SPring-8 BL08W beamline with the use of high energy (115.6 keV) synchrotron radiation.

We also present the new theoretical CP calculations based on the DTF theory, where calculations were carried out within the full potential (linearized) augmented plane wave method with local orbitals (FP-LAPW+lo).

We observed a significant improvement of the agreement between experimental and theoretical CP anisotropies compared to the previous results (Fig. 1). Despite the differences observed between both, KKR and DFT calculations it is difficult to say unequivocally which theory describes the data more adequately.

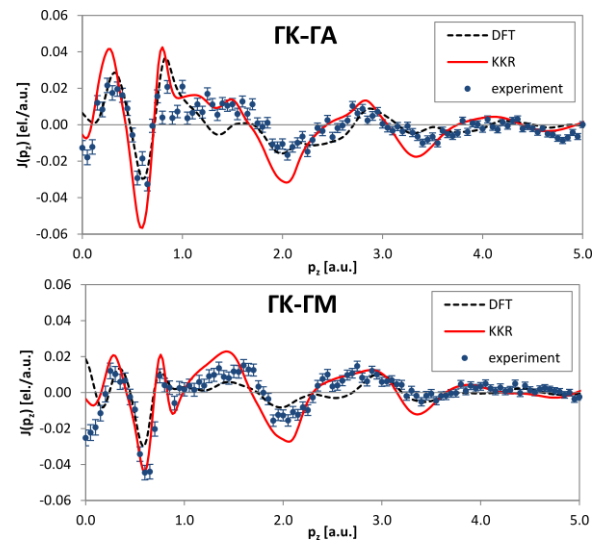


Figure 1. Two examples of directional Compton profile anisotropy measured along the three high-symmetry directions ΓA , ΓK and ΓM . Dashed and solid lines represent theoretical DFT and KKR calculations respectively, convoluted to 0.12 a.u. resolution of the experiment plotted by solid circles.

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