New Understanding of Photoelectron Diffraction: Experiment

Gerd Schönhense

Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany

Email: schoenhe@uni-mainz.de

Abstract. Photoelectron diffraction (PED), which was first developed in the 1970s [1,2], has become a powerful technique for analysing the structure of solids. Recording efficiency has been greatly improved by a full-field imaging approach, and extending into the hard X-ray region provides access to true bulk information [3]. In this study, we present a novel application of PED at extremely low kinetic energies, within the range of the minimum inelastic mean free path curve [4]. Measurements were performed at beamline I09 of the Diamond Light Source (Harwell Campus, UK). The soft X-ray branch houses a unique momentum microscope that combines a large hemispherical analyser with time-of-flight detection. This allows the simultaneous acquisition of $I(E_B,k_x,k_y)$ data arrays [5].

A full-field PED pattern with a diameter of ~7 Å^{-1} is typically acquired in 5-10 minutes. This high recording speed enables ***PED movies*** to be captured with small kinetic energy steps down to 2 eV. Such movies have been recorded for Si 2*p,* Ge 3*d* and Ge 3*p* core-level photoelectrons at final state energies between 45 and 400 eV (kinetic energy inside the material). Thanks to a novel type of objective lens [6], these patterns correspond to polar angle ranges of 0-90° at 45 eV and 0-30° at 230 eV. The richness in detail is incompatible with the low IMFP in this energy range. Fig. 1 shows different sections through such a 3D stack for Si 2$p_{3/2}$; the image contrast is CDAD. Understanding these patterns requires new concepts to describe the core-level photoemission process, particularly with regard to the nature of the final state (see the talk by Jan Minar).

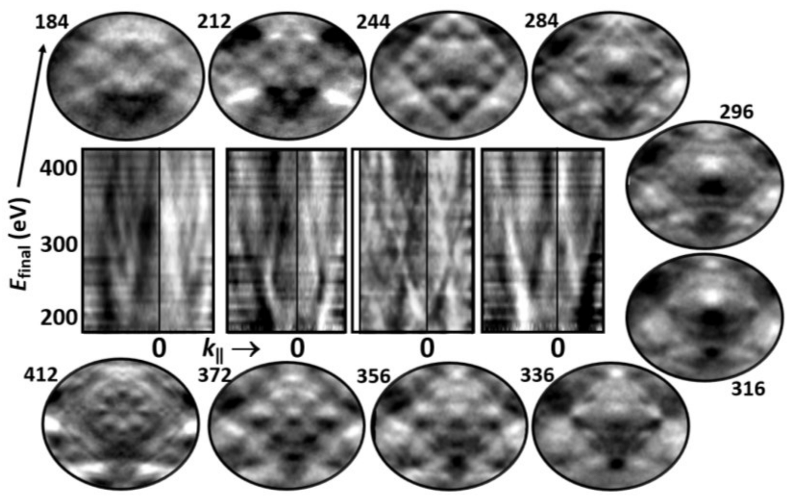

Figure 1. PED measurement (CDAD contrast) for Si 2$p_{3/2}$, recorded in a photon energy range from 270 to 500 eV. The outer panels show k_x-k_y sections, the inner ones E_B-*vs*-$k_{parallel}$ sections at different positions. E_{final}= h*ν*-E_B+V_0 is the kinetic energy inside of the solid. (from [7])

References:

[1] K. Siegbahn et al., *Phys. Scripta* **1**, 272 (1970).
[2] C. S. Fadley & S. A. L. Bergstrom, *Phys. Lett.* A **35**, 375 (1971).
[3] O. Fedchenko et al., *J. Phys. Society Jap.* **91**, 091006 (2022); doi:10.7566/JPSJ.91.091006
[4] M. P. Seah & W. A. Dench. *Surf. Interface Analysis* **1**, 2-11 (1979); doi:10.1002/sia.740010103.
[5] M. Schmitt et al., *Ultramicroscopy* (2025); doi: 10.1016/j.ultramic.2025.114169
[6] O. Tkach et al., *Ultramicroscopy* (2025); doi:10.1016/j.ultramic.2025.114167
[7] O. Tkach, D. Biswas, J. Liu, T.-L. Lee, H.-J. Elmers and G. Schönhense, *in preparation*