New Understanding of Photoelectron Diffraction: Experiment

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Abstract. Photoelectron diffraction (PED), initiated by pioneering work in the 1970s [1,2], has developed into a powerful technique for the structural analysis of solids. Recording efficiency has been greatly improved by a full-field imaging approach, and the extension into the hard X-ray region provides access to true bulk information [3]. Here we discuss a novel aspect of PED at very low kinetic energies in the range of the minimum of the inelastic mean free path IMFP curve [4]. The measurements were performed at beamline I09 of the DIAMOND Light Source (Harwell Campus, UK). The low-energy branch of I09 houses a novel hybrid momentum microscope combining a large hemispherical analyzer (225 mm radius) with time-of-flight detection, allowing 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 allows capturing ***PED movies*** with small steps of the kinetic energy down to 2 eV. We have recorded such movies for Si 2*p,* Ge 3*d* and Ge 3*p* core-level photoelectrons at final state energies between 45 and 230 eV (kinetic energy inside of the material) [6]. In real-space coordinates (the usual way of presenting PED data) these patterns correspond to polar angle intervals ranging from 0-90° at 45 eV to 0-30° at 230 eV. The patterns are rich in detail and are incompatible with the low IMFP in this energy range. Understanding their fine structure requires new concepts of the solid-state photoemission process, especially with respect to the nature of the final state.

[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*, in print (2025); e-print on arXiv 2406.00771.
[6] O. Tkach, D. Biswas, J. Liu, T.-L. Lee, H.-J. Elmers and G. Schönhense, *in preparation*