

## Electronic structure determination by means of the momentum microscope

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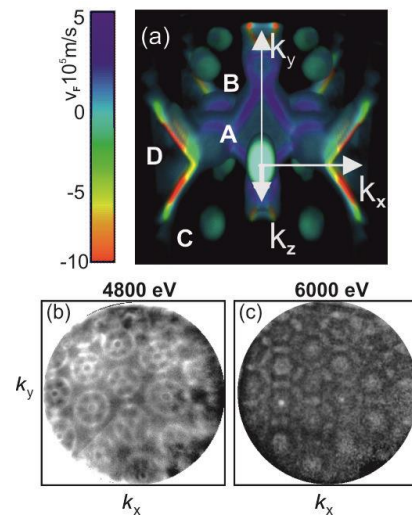
Angular- or momentum-resolved photoelectron spectroscopy in the Soft and Hard X-ray ranges is a major tool for studying the electronic structure of solids. Information depths of several nm give access to the bulk momentum-resolved structure in the valence range using conventional spectroscopy [1] and  $k$ -microscopy [2]. With increasing probing depth, the relative contribution of the surface is decreasing so it gives access to the bulk bands in particular for reactive samples and unprepared or coated surfaces. In my talk I will mainly concentrate on the ongoing development at University of Mainz in the field of time-of-flight (ToF)  $k$ -microscopy in the Soft and Hard X-ray ranges.

Experimental data at photon energies up to 1700 eV were obtained at beamline P04 (PETRA III, Hamburg, Germany) by a full mapping of the bulk electronic structure including the Fermi surface and Fermi-velocity distribution  $v_F(k_F)$  (Fig. 1a) of tungsten [3]. The 4D spectral function  $\rho(E_B; k)$  in the entire bulk Brillouin zone and 6 eV binding-energy ( $E_B$ ) interval was acquired in  $\sim 3$  hours thanks to a new multidimensional photoemission data-recording technique (combining full-field  $k$ -microscopy with ToF parallel energy recording) and the high brilliance of the soft X-rays used. A direct comparison of bulk and surface spectral functions (taken at low photon energies) reveals a time-reversal-invariant surface state in a local bandgap in the (110)-projected bulk band structure.

Recently, we have extended the same approach to hard-X-ray photoelectron spectroscopy (HAXPES). Construction of a  $k$ -microscope with a modified lens system, optimized for high kinetic energies ( $> 8$  keV) with high angular resolution  $< 0.1^\circ$  and very large field of view in  $k$ -space (up to  $20 \text{ \AA}^{-1}$  diameter) [4]. Combining the large  $k$ -space acceptance of the special objective lens for simultaneous full-field imaging of many Brillouin zones with ToF energy recording yields maximum parallelization. Thanks to the high brilliance ( $10^{13} \text{ hv/s}$  in a spot of  $< 20 \text{ \mu m}$  dia.) of beamline P22 (PETRA III, Hamburg, Germany) the microscope set a benchmark in HAXPES recording speed. Count rates reached several million counts per second for core-level signals and  $d$ -bands of transition metals. The concept of tomographic  $k$ -space mapping established using soft X-rays works equally well in the hard X-ray range. Experimental data reveal sharp valence band  $k$ -patterns, e.g. for Re (Fig. 1b,c) showing 19 Brillouin zones in parallel. The pattern at an excitation energy of 6 keV corresponds to direct transitions to the 28th repeated Brillouin zone along  $k_z$ . X-ray photoelectron diffraction (XPD) patterns with  $< 0.1^\circ$  resolution and unprecedented rich fine structure are recorded within minutes. The short photoelectron wavelength (10% of the interatomic distance) “amplifies” phase differences and will make full-field hard X-ray XPD a very sensitive structural tool.

### References

- [1] A. X. Gray et al. *Nature Materials* **10**, 759 (2015).
- [2] G. Schönhense et al., *JESRP* **200**, 118 (2012).
- [3] K. Medjanik et al., *Nature Materials* **16**, 615 (2017).
- [4] K. Medjanik et al., arXiv:1810.11366 (2018).



**Fig. 1:** (a) Fermi surface and Fermi velocity (color bar) of tungsten (from [3]), (b,c)  $k$ -space map for the  $d$ -bands of Re taken at  $h\nu = 3800$  and  $6000$  eV ( $T \sim 20$  K), from [4].