k-resolved electronic structure by soft-X-ray ARPES: From 3D systems to buried interfaces and impurities

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The spectroscopic power of soft-X-ray ARPES (SX-ARPES), employing photon energies hv around 1 keV, arises from an increase of the photoelectron escape depth by a factor of 3-5 compared to the conventional VUV-ARPES, concomitant sharp definition of the 3D electron momentum **k**, and resonant photoexcitation delivering elemental and chemical state specificity. Recently, the advanced instrumentation at the Swiss Light Source has allowed SX-ARPES to develop from the traditional applications to 3D bulk crystals to photon-hungry cases of buried interfaces and impurities. In this talk, I unfold this development vector with a series of recent highlights [1].

3D materials. Applications to 3D materials are illustrated, for example, by the Fermi surface (FS) of the transition metal dichalcogenide VSe₂ measured at hv around 1 keV (Figure). Improved definition of 3D momentum results in textbook clarity of the experimental FS. Its autocorrelation analysis reveals an out-of-plane nesting which acts as the precursor for the exotic 3D charge density waves. Other examples include modulated FS shapes in pnictide HTSCs caused by their 3D character and intra-cell interference effects, bulk Rashba splitting in noncentrosymmetric topological insulator BiTeI, bulk FS of the pseudocubic perovskite La_{1-x}Sr_xMnO₃ with characteristic features manifesting the rhombohedral structural distortion related to the CMR, 3D Fermi states of quasicrystalline AlNiCo, etc.



Buried interfaces. Experiments on the LaAlO₃/SrTiO₃ conducting interface exploited resonant photoexcitation of the interface Ti³⁺ ions to accentuate the signal from the buried interface carriers. Using variable X-ray polarization, we have resolved different subbands of the interface quantum well states resonating in different surface Brillouin zones. Luttinger count of the experimental FS goes along with the experimental carrier concentration with deviations hinting at various carrier localization mechanisms. The d_{xy} -subbands with their strong interface confinement show a peak-dip-hump spectral function characteristic of polaronic coupling.

Buried impurities. Resonant SX-ARPES applied to the paradigm diluted magnetic semiconductor GaMnAs has identified the ferromagnetic Mn impurity band, and established its energy alignment and mechanism of hybridization with the host GaAs bands. Combining the previous *p-d* exchange and double-exchange models, these results suggest a microscopic picture of the GaMnAs ferromagnetism based on the Anderson impurity model. Another example in this field is InFeAs showing the ferromagnetism induced by doped electron carriers.

[1] V.N. Strocov et al, Synchr. Rad. News 27, N2 (2014) 31