Photoelectron diffraction for probing structural, electronic and magnetic properties of 4f materials

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Photoelectron diffraction (PED) is well established as an efficient method for structural analysis of crystalline surfaces, defects and impurities, thin films, adsorbates, 2D materials, and other systems [1]. It is based on the fact that photoelectrons emitted from the atomic sites, called emitters, experience multiple scattering on the surrounding atoms when they propagate to the sample surface. As a result, the angular distribution of the measured photocurrent represents a diffraction pattern, which contains information about the local environment of the emitters. In a common PED experiment, electrons are emitted from the closed core shell, leaving the atom with a core hole. Interactions of the core hole with valence electrons may give rise to several spectral components, known as the atomic multiplet. The photoemission intensities of the multiplet components are sensitive to the local magnetic order in the system even in the absence of net magnetization, enabling PED-based insight into magnetic phase transitions in the near-surface region. Nonradiative decay of the core hole produces Auger electrons, giving rise to a so-called Auger electron diffraction. Both direct photoemission and Auger processes can be combined to selectively increase the signal from the atoms of interest by an order of magnitude or even more. This is realized in resonant PED experiments, when the photon energy is selected close to the absorption edge of a core shell, being particularly useful for studies of impurities and defects at low concentrations.

Here, we will consider the applications of PED in the structural studies of graphene-based systems and magnetic topological insulators. While PED became a routine technique when based on photoemission from a closed shell, it may also be also of interest to consider emission from an open shell. This is of particular importance for studies of materials containing lanthanides. Here, we demonstrate a methodology of PED experiments with the aim to study the properties of 4f materials. Some of these materials exhibit strongly correlated electronic behavior and unusual magnetic properties. Our results demonstrate that the capabilities of photoelectron diffraction extend far beyond the crystal structure analysis, allowing to study the changes in the valency of 4f elements, the directions of magnetic moments, the differences in the magnetic properties of the surface layers relative to the bulk ones, and the ground state of 4f shell split in the crystal electric field [2-4].

The work was supported by the Ministry of Science and Higher Education of the Russian Federation (No. 075-15-2025-010) and by the St Petersburg State University (Grant No. 125022702939-2).

Bibliography

[1] M.V. Kuznetsov et al. J. Phys. Soc. Japan 87, 061005 (2018)
[2] D.Yu. Usachov et al. Phys. Rev. B 102, 205102 (2020)
[3] D.Yu. Usachov et al. J. Phys. Chem. Lett. 14, 5537 (2023)
[4] D.Yu. Usachov et al. Phys. Rev. B 109, L241118 (2024)