Analyzing Core Level Photoelectrons by Diffraction and Circular Dichroism Via Means of First-Principle Scattering Calculations

Trung-Phuc Vo[1, 2, a)], Olena Tkach[3, 4], Sylvain Tricot[5], Didier Sébilleau[5], Aimo Winkelmann[6], Olena Fedchenko[3], Yaryna Lytvynenko[3, 7], Dmitry Vasilyev[3], Hans-Joachim Elmers[3], Gerd Schönhense[3], and Ján Minár[1, b)]

[1]*New Technologies-Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic.*
[2]*Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czech Republic.*
[3]*Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany.*
[4]*Sumy State University, Rymskogo-Korsakova 2, 40007 Sumy, Ukraine.*
[5]*Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000, Rennes, France.*
[6]*AGH University of Krakow, Academic Centre for Materials and Nanotechnology, Kraków, Poland.*
[7]*Institute of Magnetism of the NAS of Ukraine and MES of Ukraine, 03142 Kyiv, Ukraine.*

[a)] Corresponding author: votrung@ntc.zcu.cz
[b)] jminar@ntc.zcu.cz

Abstract. Photoelectron diffraction (PED) of core-level photoemission is an influential spectroscopic technique that provides valuable insights into the electronic and geometrical structure of materials at the atomic scale. In fact, it is not only a powerful method but also an unexpected effect. The choice of an appropriate theoretical formalism to interpret the experiments is therefore a necessity. Building on our previous successful work on the implementation of PED under the SPRKKR package, this study presents new and detailed experimental-theoretical comparisons of other core levels, providing deeper insights into material properties. We have calculated the circular dichroism in angular distributions (CDAD) for 3p, 3d and 4p of W(110) for application-specific purposes. The discriminant diffractogram between split core-levels is discussed. Hard X-rays (6000~eV) with right and left circularly polarized radiation (RCP and LCP, respectively) are used to generate photoelectrons. Through a comprehensive comparison of measured and calculated results, this study advances our understanding of PED simulations and their implications for materials characterization and discovery.

ACKNOWLEDGMENTS

This work was supported by the project Quantum materials for applications in sustainable technologies (QM4ST), funded as project No. CZ.02.01.01/00/22 008/0004572 by Programme Johannes Amos Commenius, call Excellent Research (J.M., T.-P.V.) and the Czech Science Foundation Grant No. GAČR 23-04746S (T.-P.V.). This work was also supported by the Deutsche Forschungsgemeinschaft, Grant No. TRR288–422213477 (Project B04), and by the Federal Ministry of Education and Research (BMBF, Project 05K22UM2).