Unveiling Fine Structure and Energy-Driven Transition of Photoelectron Kikuchi Diffraction

Trung-Phuc Vo[1,2], Olena Tkach[3,4], Aki Pulkkinen[1], Didier Sebilleau[5], Aimo Winkelmann[6], Olena Fedchenko[3], Yaryna Lytvynenko[3,7], Dmitry Vasilyev[3], Hans-Joachim Elmers[3], Gerd Schönhense,[3] and Jan Minar[1, a)]

[1]New Technologies-Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic.
[2]Institute of Physics, Czech Academy of Sciences, Cukrovarnicka 10, 162 00 Praha6, Czech Republic.
[3]Johannes Gutenberg-Universitat, Institut fur 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, Krakow, Poland.
[7]Institute of Magnetism of the NAS of Ukraine and MES of Ukraine, 03142 Kyiv, Ukraine.

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

Abstract. The intricate fine structure of Kikuchi diffraction plays a vital role in probing phase transformations and strain distributions in functional materials, particularly in electron microscopy. Beyond these applications, it also proves essential in photoemission spectroscopy (PES) at high photon energies, aiding in the disentanglement of complex angle-resolved PES data and enabling emitter-site-specific studies. However, the detection and analysis of these rich faint structures in photoelectron diffraction (PED), especially in the hard X-ray regime, remain highly challenging, with only a limited number of simulations successfully reproducing these patterns [1,2]. The strong energy dependence of Kikuchi patterns further complicates their interpretation, necessitating advanced theoretical approaches. To enhance structural analysis, we present a comprehensive theoretical study of fine diffraction patterns and their evolution with energy by simulating core-level emissions from Ge(100) and Si(100). Using multiple-scattering theory and the fully relativistic one-step photoemission model [3-5], we simulate faint pattern networks for various core levels across different kinetic energies (106 eV - 4174 eV), avoiding cluster size convergence issues inherent in cluster-based methods. Broadening in patterns is discussed via the inelastic scattering treatment. For the first time, circular dichroism has been observed and successfully reproduced in the angular distribution of Si (100) 1s, revealing detailed features and asymmetries up to 31%. Notably, we successfully replicate experimental bulk and more ”surface-sensitivity” diffraction features, further validating the robustness of our simulations. The results show remarkable agreement with the experimental data obtained using circularly polarized radiations, demonstrating the potential of this methodology for advancing high-energy PES investigations.

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