New Understanding of Photoelectron Diffraction: Theory

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Abstract. Photoelectron diffraction (PED) is a powerful and indispensable experimental technique for resolving the structure of surfaces with sub-angstrom resolution. In many instances, it provides structural insights related to element specificity [1], which is essential for understanding phenomena related to electronic properties. In the high-energy regime, angle-resolved photoemission spectroscopy (ARPES) often reveals PED effects, accompanied by challenges such as small cross-sections, significant photon momentum transfer, and non-negligible phonon scattering [2]. Overall, X-ray PED (XPD) is not only an advantageous approach but also exhibits unexpected effects. Powerful computational approaches that address single and multiple scattering in real space and reciprocal space have been developed earlier. However, they do share limitations related to angular momentum, cluster size and constrain in kinetic energy regimes. To overcome these barriers and disentangle diffraction effects, we present a PED implementation [3] for the SPRKKR package that uses multiple scattering theory and a one-step model [4,5]. in the photoemission process. In contrast to real-space implementations of the multiple scattering XPD formalism, we propose a k-space implementation based on the layer KKR method. The main advantage of this method is its ability to address a very broad kinetic energy range (20-8000 eV) without convergence problems related to. The inelastic scattering is investigated as a broadening mechanism. Furthermore, the so-called alloy analogy model can be used to simulate XPD at finite temperatures as well as XPD effects observed in soft and hard X-ray ARPES. Here, the brief summary of theoretical models and practical applications [6,7] for core-level photoemission is addressed.

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