

Circular dichroism by core-level angle-resolved photoemission: Application of multiple&single-site scattering theory

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Photoelectron diffraction (PED) is a powerful and driving experimental technique for resolving the structure of surfaces with sub-ångstrom resolution. Being able to opt the emitters based on their specific binding energy makes PED widely used for following investigation purposes: crystal structures, bonding geometries of atoms and the local environment of impurity or dopant atoms inside surfaces [1]. Similarly, to angle-resolved photoemission spectroscopy (ARPES), the angular distribution of photoelectrons emitted from a crystal surface is studied. Nevertheless, the physics behind and investigation objective are distinct for two mentioned approaches. The angular distribution of emitted electrons represents the momentum of initial states in ARPES meanwhile it reveals the interference of photoelectron waves from final states in PED. Depending on the utilized photon energies, this tool can be termed either ultraviolet-PED (UPD) or X-ray-PED (XPD). In high energy regime, XPD effects are found in ARPES measurements beside other obstacles (low cross-sections, large photon momentum transfer, non-negligible phonon scattering) [2]. Overall, XPD is not only an advantageous approach but also an unexpected effect [3]. Here, to disentangle these diffraction influences, we present a PED implement for SPRKKR package [4] which makes use of multiple scattering theory and one-step model in photoemission process [5].

In contrast to the other real space implementations of the multiple scattering XPD formalism, here we propose to use k-space implementation based on the layer KKR method. Main advantage of this method is that we can without convergence problems (wrt. the angular momentum and cluster size) address very broad kinetic energy range (20-8000eV). Furthermore, the so-called alloy analogy model [6,7] can be used to simulate XPD at finite temperatures as well as XPD effects observed in the soft and hard X-ray ARPES [8]. For the sake of applications, we have calculated the circular dichroism in angular distributions (CDAD) associated with core-level photoemission of 3d from W(110) and 3p from Ge(100) [9]. Photoelectrons are excited by hard X-rays (6000 eV) with right and left circularly polarized radiation (RCP and LCP, respectively).

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