Circular Dichroism in Angle-Resolved Photoemission from Core-Level Emission of W(110)

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Abstract. Angle-resolved photoemission spectroscopy (ARPES) is a powerful and driving experimental technique for examining the electronic structure of quantum materials [1]. Advanced developments consisting of new photon sources, analyzers and detectors considerably enhance the resolution of spin, angle and energy [2,3]. There is another technique called X-ray photoelectron diffraction (XPD) which is considered to be the same thing as ARPES from an elementary point of see, specifically the angular distribution of photoelectrons emitted from a crystal surface. 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 XPD. At high photon energies, photoelectron diffraction (PED) effects are found in ARPES measurements beside other obstacles (low cross-sections, large photon momentum transfer, non-negligible phonon scattering) [4]. Here, to disentangle these diffraction influences, we present a PED implement for SPRKKR package which makes use of multiple scattering theory and one-step model in photemission process [5,6,7]. For the sake of applications, we have calculated the circular dichroism in angular distributions (CDAD) associated with core-level photoemission of 4f and 3d from W(110). Photoelectrons are excited by hard X-rays (6000 eV) with right and left circularly polarized radiation (RCP and LCP, respectively).

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