Angle-resolved photoemission of noble metals in the X-ray regime

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The angle-resolved valence band photoemission of noble metals in the X-ray regime has been studied by means of the one-step model of photoemission. For this purpose the fully relativistic version of the multiple scattering or Korringa-Kohn-Rostoker (KKR) formalism has been used. This very powerful approach allowed in particular to account for the impact of spin-orbit coupling on the polarisation dependence of the resulting spectra. All calculations are based on the use of a ground state potential determined in a self-consistent way within the framework of local density approximation (LDA). To account for finite lifetime effects a suitable complex self-energy has been added. For the X-ray regime, it could be demonstrated that the so-called single-scatterer approximation for the final states is a very good approximation. This implies in addition that surface effects are in general of minor importance. Our theoretical results are directly compared to corresponding experimental spectra recorded recently at the ESRF. In general a very satisfying agreement is found. This applies in particular to the polarization dependence of the spectra. Apart from a detailed comparison of the theoretical and experimental spectra the applicability of a free-electron parabola for the reconstruction of the dispersion relation E(k) will be discussed.