

Nature of photoemission in the range of the 5s-photoelectron spectrum of iridium

A.T. Kozakov¹, A.V. Nikolsky¹, K.A. Googlev¹, I.D. Petrov², B.M. Lagutin², V.L. Sukhorukov¹,
H. Huckfeldt^{3,4}, D. Holzinger^{3,4}, A. Gaul^{3,4}, and A. Ehresmann^{3,4}

¹*Institute of Physics, Southern Federal University, 344090, Rostov-on-Don, Russia*

²*Rostov State Transport University, 344038, Rostov-on-Don, Russia*

³*Institut für Physik, Universität Kassel, D-34132 Kassel, Germany*

⁴*Center for Interdiscipl. Nanostruct. Sci. and Technology, D-34132 Kassel, Germany*

Presenting Author: sukhorukov_v@mail.ru

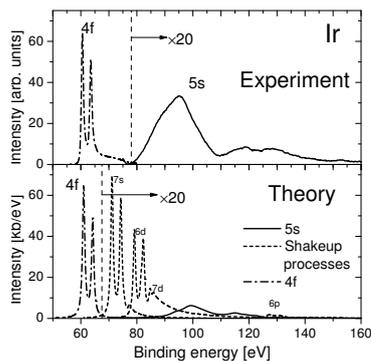


Figure 1: Photoelectron spectrum of 4f- and 5s-shells of Ir. Intensity of the spectra is scaled by 20 at the right side of the vertical dashed line.

The 4f and 5s X-ray photoelectron spectra (XPES) of the iridium metal excited by monochromatized Al K_{α} radiation were measured using the X-ray photoelectron microprobe ESCALAB-250. These spectra are presented in the upper panel of Fig. 1. The integral intensity of the measured 5s spectrum amounts to 21.7% of the 4f spectrum intensity, whereas the estimate using the Hartree-Fock-Slater data of Yeh and Lindau [1] yields for this ratio about 3% only.

In the present work we calculated the 4f and 5s XPES of Ir using the configuration interaction Pauli-Fock approximation with core polarization (CIPFCP) [2]. The spectra were computed applying the isolated-atom model. The 5s XPES was computed in the $5s^25p^65d^76s^2(^4F_{9/2})$ ground state, whereas in the calculation of the 4f XPES the 5d-shell was treated as a spherical one. The most important many-electrons effects influencing the 5s- ϵp photoemission were found to be: (i) dipole polarization of electron shells (DPES), described by the $5p5p-5s5d$, $4f5p-5s5d$ and $4f4f-5s5d$ excitations of the $5s^15d^7$ ionic state and contributing multiplet structure of the 5s XPES; (ii) intershell correlations described by the interaction between the 5s- ϵp , 4f- $\epsilon(d/g)$, and 5p- $\epsilon(s/d)$ channels and contributing about 3% to the 5s- ϵp photoionization cross section; (iii) double-electron single-photon correlational transitions $4f5p-5d\epsilon\ell$ ($\ell = 1, 3, 5, 7$) through the $4f^{13}5p^65d^7\epsilon'\ell'$ intermediate channels contributing satellites which have binding energies in the range of 110-140 eV and 16% of the 5s XPES intensity.

Computed 4f and 5s XPES are presented in the lower panel of Fig. 1. For better clarity, the theoretical binding energies were decreased by 9 eV. The integral intensity of the computed 5s XPES amounts to 3.4% only of the 4f XPES intensity. We suppose that the 5s-photoionization is not a dominant process forming the spectrum in the 80–140 eV energy range. In order to reveal an additional mechanism of the photoemission in this energy range, we calculated the shake excitation/ionization processes of the outer 5p-, 5d- and 6s- electrons accompanied by creation of the 4f vacancy. They were calculated within the sudden approximation and are presented in the lower panel of Fig. 1 by dashed curves. The integral intensity of the XPES in the 5s-energy range amounts to 18,6% of the 4f-XPES intensity, which is close to the experimental value. However, the shape of the theoretical spectrum differs from the experimental one. This discrepancy can be connected with the limitations of the isolated-atom model.

References

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- [2] V. L. Sukhorukov *et al.* *J. Phys. B: At. Mol. Opt. Phys.* **45** 092001 (2012)