Journal of Physics: Conference Series **488** (2014) 022044 doi:10.1088/1742-6596/488/2/022044

On Photoionization in the Hard X-Ray Region

M. Ya. Amusia*† [1], L. V. Chernysheva†, and V. G. Yarzhemsky††

* Racah Institute of Physics, Hebrew University, Jerusalem, 91904, Israel
† Ioffe Physical-Technical Institute, RAS, St. Petersburg, 194021, Russia
†† Kurnakov Institute of General and Inorganic Chemistry, Moscow, 119991, Russia

Synopsis It is demonstrated that recent experiments on ionization of 3p and 3s electrons in Ni film and solid body [1] cannot be described in the frames of Hartree-Fock or the random phase approximation with exchange. The deviation is so big that from the theoretical side it requires inclusion of huge and yet unknown effects

1. Recently the first measurements were performed of the ionization cross-section by photons in the frequency range $\omega = 2-9keV$ on 3s and 3p subshells of Ni thin films and crystals [1]. The results were compared to old calculations [2], and an essential difference particularly for the 3s subshell in the high frequency region was found. It appeared that the measured cross-section is smaller than the calculated one by a factor 2.5. An essential difference was observed between thin films and crystals, which is surprising since the ionization potentials of 3s and 3p are much bigger than the typical solid body binding energies and much smaller than ω.

2. It was demonstrated in [3] that the corrections of the random phase approximation with exchange (RPAE) are important even in the high photon energy limit. They are powerful enough even to alter the cross-section behavior at $\omega \to \infty$. So, it was quite natural to apply the RPAE approach to reproduce the data from [1].

3. It is essential that the measurement was performed at such an angle that the really obtained quantity was not the photoionization cross-section $\sigma_{3s,3p}(\omega)$ but $\sigma_{3s,3p}(1+\beta_{3s,3p})$, where $\beta_{3s,3p}$ are the dipole angular anisotropy parameters of 3s and 3p subshells, respectively. The non-dipole parameters on the base of previous calculations were assumed to be small in the studied ω region.

4. So, we have calculated the cross sections and angular anisotropy parameters, dipole and non-dipole, in the frame of one electron Hartree-Fock (HF) approach and with account of RPAE multi-electron correlations. It appeared that in the region of interest, dictated by [1], the contribution of the non-dipole parameters is small indeed. The dipole parameters as well as cross-sections proved to be almost the same in HF and RPAE, thus signaling that the role of RPAE corrections is small enough.

5. Figure 1 shows the result obtained for the ratio $\sigma_{3s}(1+\beta_{3s})/\sigma_{3p}(1+\beta_{3p})$, both measured and calculated. On the same Figure we present results of [2] and in HF – Slater approximation

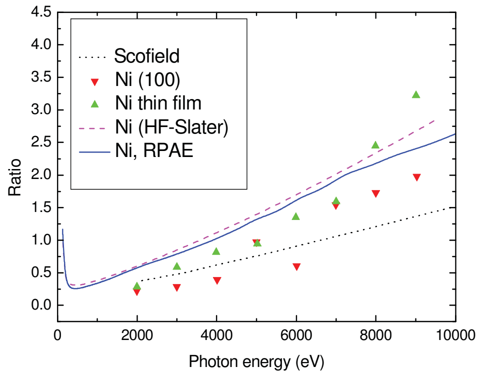

Figure 1. The results of measurement [1] and calculation for the ratio $\sigma_{3s}(1+\beta_{3s})/\sigma_{3p}(1+\beta_{3p})$ in Ni film and crystal.

6. Neither HF nor RPAE are able to describe the experimental data for the absolute values of the cross-sections or, as is seen in Figure 1, in the ratio. The difference is quite large. It surprises the strong influence of the shape of the sample – is it a crystal or a film. Further theoretical and experimental studies are desirable in this promising direction.

References

[1] A. M. Gorgoi *et al*. J. Elect. Spect. & Related Phenomena 2013 http://dx.doi.org/10.1016/j.elspec.2013.01.
[2] J. H. Scofield 1973. LLNL report UCRL-51326
[3] M. Ya. Amusia *et al* 2000. *Phys. Rev. Lett.* 85, 4703.

† [1] E-mail: amusia@vms.huji.ac.il