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Report:

Indroduction

Double photoionization (DPI) leading to an empty 1s shell serves as one of the most sensitive probes of electron-electron correlations. The ejection of two electrons would not occur in the independent electron picture. Thus, the double-to-single 1s photoionization cross-section ratio σ_{KK}/σ_K permits to quantify electron-electron correlations. Following the absorption of the primary photon, two dominant mechanisms produce "hollow atoms", namely the shake process (SO) and the electron-electron scattering (two-step-one TS1). In shake-off the primary electron is ejected rapidly and the resulting sudden change of the atomic potential leads to a subsequent removal of the second photoelectron to the continuum. In the TS1 process, the first electron knocks out the second one in an (e,2e) like electron impact “half-collision”. The initial-ground-state correlations are probed by the shake process, while the final-state electron interactions govern the TS1 mechanism. It is difficult to distinguish between the two processes, and the relative importance of the two mechanisms at different photon energies has been well quantified only for He [1,2]. The importance of the dynamical electron-electron scattering contribution with increasing Z has been recognized quite recently [3]. In fact, for elements other than He, the double-to-single 1s photoionization cross-section ratio P_{KK} has been measured solely from threshold for double ionization to the broad maximum, but not beyond [3-6].

We report on the photon energy-dependence of the double-to-single K-shell photoionization ratio P_{KK} for low-Z elements Mg, Al and Si investigated by means of high-resolution x-ray emission spectroscopy. The P_{KK} values for photon energies beyond the maximum were obtained. These are the first measurements of this kind. The evolution of the dynamical electron-electron scattering contribution to the DPI cross-section could be assesed.

Experiment

The double K–shell vacancy production was studied by means of high-resolution x-ray emission spectroscopy. Measurements of the $K^{-2} \rightarrow K^{-1}L^{-1}$ hypersatellite $K\alpha_2^h$ and diagram $K\alpha$ x-ray spectra were carried out at the ESRF ID26 beam line using the high-resolution von Hamos Bragg curved crystal x-ray spectrometer of Fribourg [7] (see Fig.1). The x-ray emission spectra of Mg were measured using a TlAP(001) crystal (2d = 25.772 Å) in second order and those of Al and Si with an ADP(101) (2d =10.642 Å) crystal in first order.

Fig. 1. Photograph of the von Hamos specrometer installed at the ESRF beamline ID26.

The diffracted x-rays were recorded with a 26.8 mm long and 8 mm high position-sensitive back-illuminated CCD detector consisting of 1340 columns and 400 rows with a pixel size of 20x20 μm^2. The CCD detector was cooled thermo-electrically to -50°. Self-supported 3.3 μm and 50 μm thick metallic foils of Mg, a 1 μm thick foil of Al and a 1mm thick c-Si sample were used. The energy calibration and the instrumental response of the crystal spectrometer were determined from the measurements of the Kα x-ray lines of Mg, Al and Si, and the $L\beta_1$ lines of Se and Ag. The instrumental response function of the spectrometer was found to be well reproduced by a Lorentzian profile with a width (FWHM) of 0.54(1) eV at the energy of the Mg K-hypersatellite line and a Gaussian profile width (FWHM) of 0.32(1) eV and 0.40(1) eV for the Al and Si K-hypersatellite line, respectively. The double-crystal Si(111) monochromator was employed and the Si coated and Cr coated double mirrors were used for harmonic rejection. The beam was focused horizontally to 250 μm at the sample thereby permitting to operate the spectrometer in the so-called slit-less geometry leading to a higher overall detection efficiency. The incident photon flux was $\sim$1-3×10^{12} ph/s depending on the photon energy.

Data analysis and Results

For illustration, the high-resolution K-hypersatellite ($1s^{-2} \rightarrow 1s^{-1}2p^{-1}$) x-ray emission spectra of Si are shown in Fig.2. Since for light elements the L-S coupling scheme prevails, the spin-flip $K\alpha_1^h$ transition ($^3P_1 \rightarrow {}^1S_0$) is dipole-forbidden. As a consequence, the $K\alpha_1^h$ line is very weak and could be only observed for Si. The Si K-hypersatellite x-ray emission line is accompanied by L-satellites resulting from the presence of the 2p and 2s vacancies during the x-ray transition. In addition, on the low energy side of the $K\alpha_2^h$ x-ray line the $K\beta L^1$

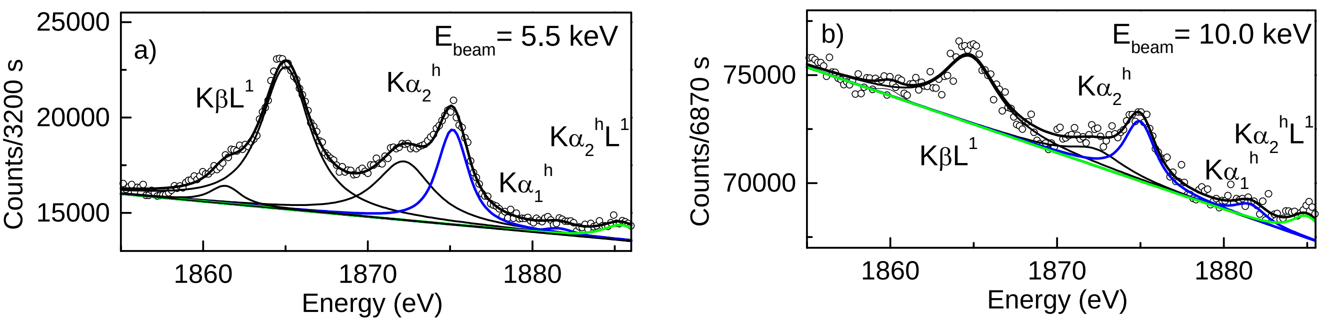

Fig. 2. High-resolution K-hypersatellite ($1s^{-2} \rightarrow 1s^{-1}2p^{-1}$) x-ray emission spectra of Si measured at a beam energy of 5.5 keV(a) and 10 keV (b).

($K^{-1} \rightarrow L^{-1}M^{-1}$) satellite transitions can be seen. To de duce the intensities, linewidths and energies of the K-hypersatellite lines, Lorentzian profiles were used to fit the measured spectra of Mg and Voigt functions for Al and Si spectra. The obtained x-ray line intensities were corrected for sample self-absorption and absorption of the incident x-rays, the photon flux, the spectrometer solid angle, as well as for the CCD quantum efficiency.

In order to probe the evolution of the double ionization probability as a function of the excitation photon energy, the $K\alpha_{1,2}$ and $K\alpha_2^h$ x-ray transitions were measured at different incident beam energies. Since for Mg and Al data for photon energies from the DPI threshold to the maximum were already collected at the ID21 beamline [reports HS-2934 and HS-2404], x-ray emission spectra for Mg were measured at 3310, 5000, 6000, 7000 and 8000 eV, and the Al x-ray spectra at 4786, 5120 and 7000 eV photon energies. For Si a complete set of data points for twelve beam energies from 3.6 keV to 10.0 keV was obtained. Due to a decrease of the σ_K and σ_{KK} cross-sections with photon energy and a quite high background, x-ray hypersatellite spectra could not be measured at higher energies.

The ratio of double-to-single K-shell ionization by photoabsorption P_{KK} was determined from the relative intensities I of the $K\alpha_2^h$ and $K\alpha_{1,2}$ x-ray emission lines employing the expression:

$$P_{KK} = \frac{\omega_K I_{K\alpha^h}}{\omega_{KK} I_{K\alpha}}$$

where ω_K and ω_{KK} are the fluorescence yields for the single- and double-hole state, respectively. The double to single K-shell photoionization ratios in the peak region P_{KK}^{max} were determined to be $2.03(19)\times10^{-3}$ for Mg, $1.84(20)\times10^{-3}$ for Al and 1.43(14))$\times10^{-3}$ for Si. These results are in good agreement with the $1/Z^{1.6}$-dependence of the P_{KK}^{max} of Kanter et al. [3]. From the measured data, the evolution of the dynamical electron-electron scattering contribution to the DPI cross-section of hollow low-Z atom production could be determined. First results will be published in the conference proceedings of the 21st International Conference on X-ray and Inner-Shell Processes X08, Paris, June 22-27 [8] and a manuscript is in preparation.

References

[1] T. Schneider and J.-M. Rost, *Separation and Identification of Dominant Mechanisms in Double Photoionization*, Phys. Rev. Lett. 89, 073002 (2002).

[2] A. Knapp et al*., Mechanisms of photo double ionization of helium by 530 eV photons*, Phys. Rev. Lett. 89, 033004 (2002).

[3] E. P. Kanter et al*., Double K-shell photoionization of silver*, Phys. Rev. A 73, 022708 (2006).

[4] S.H. Southworth et al., *Double K-shell photoionization of neon*, Phys. Rev A 67, 062712 (2003).

[5] R. Diamant et al., *Evolution from Threshold of a Hollow Atom's X-Ray Emission Spectrum: The Cu* $K^h\alpha_{1,2}$ *Hypersatellites,* Phys. Rev. Lett. 84, 3278 (2000).

[6] M. Oura et al., *Correlative multielectron processes in K-shell photoionization of Ca, Ti, V in the energy range of 8-35 keV*, J. Phys. B: At. Mol. Phys. 35, 3847 (2002).

[7] J. Hoszowska et al., *High resolution von Hamos crystal X-ray spectrometer,* Nucl. Instr. Meth. Phys. Res. A 376 129 (1996).

[8] J. Hoszowska et al., *Double K-shell photoionization of low-Z atoms and He-like ions,* The European Physics Journal-Special Topics, (in press).