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Threshold scan of the Ne 2s-electron photoionization cross section

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The photoionization of the Ne 2s-electrons was studied from threshold to 1 eV above threshold. The technique of photon-induced fluorescence spectroscopy was applied. Pronounced structures were observed resulting from autoionization of doubly excited atomic states. A threshold cross section of 0.17 Mb was determined.

The photoionization cross sections of the outer *n*s-electrons of the rare gases show pronounced structures near threshold. This has been demonstrated in a number of experiments of the past few years applying especially photon-induced fluorescence spectroscopy (PIFS) [1–5]. This technique decouples the bandwidth of the exciting radiation and the resolution of the fluorescence channel. It allows an unproblematic scan over an ionization threshold provided the ion is produced in an excited state. The structures in the cross sections result from the interference of the direct ionization channel with autoionization processes of doubly excited atomic states populating the $nsnp^6\,{}^2S_{1/2}$ state of the respective rare gas atom. The doubly excited states populate in a resonancelike way also the satellites as shown by PIFS [1–5,6] and in many investigations applying photoelectron spectroscopy (PES) (ref. [6], and references therein).

We have repeated a recent experiment on the 2s-electron threshold of Ne, with a five times smaller bandwidth of the exciting synchrotron radiation. The result of the earlier experiment was the first demonstration of a cross section peak at 0.5 eV above the threshold at 48.48 eV [4]. Moreover a shoulder of the cross section was indicated even closer to threshold, but the threshold value itself of the cross section was still masked. From the mentioned reduction of the bandwidth to 40 meV, a possible correlation between narrow structures observed in the total absorption cross section [7,8] and structures in the 2s-electron photoionization cross section was expected to become noticeable. Such a correlation finally has to be proven by calculations of the influence of the doubly excited states. For the Ar 3s-electron only, theoretical investigations of this influence were performed, including so far a limited number of doubly excited states of the type $ns^2np^4n'l'n''l''\ {}^1P$ [9].

The threshold scan was carried out at the synchrotron radiation facility BESSY at Berlin using a wiggler/undulator beam line with a toroidal monochromator. The photoionization process of the Ne 2s-electron was identified by observation of the $2s2p^6\,{}^2S_{1/2}$–$2s^22p^5\,{}^2P_{3/2,1/2}$ transitions at 46.1 nm using a 1 m normal incidence monochromator. The intensity of these transitions was recorded as function of the exciting photon energy, with a present integrated flux of the exciting photons driving a multiscaling system. This procedure is different from our earlier experiment where VUV fluorescence spectra were recorded by a multiplex detector with the exciting photon energy as parameter [1,4]. The spectra were analyzed later. Since only the 2s–2p transition is observed close to the 2s-electron threshold, no information is lost by the multiscaling procedure having the advantage of the evaluation of drift problems. Up to 10 scans were added. Stepwidths of 20 meV and of 10 meV were chosen. The 10 meV scan was carried out in a small energy range where most of the structures in the photoionization cross section were expected.

Figure 1 displays the result of the two mentioned scans. The data points were connected by solid lines, the 10 meV scan was shifted by 5 meV with respect to the 20 meV scan. The statistical uncertainty of the data points is in the order of the dot size, i.e. 3% around 49 eV. The relative energy scale of the experiment was put on an absolute scale by fixing the known energy value of the 2s-electron photoionization threshold at 40 meV above the sharp rise of the signal. This was justified by the observed bandwidth of the exciting radiation of 40 meV, a value which was derived from the halfwidth of the peak structure at the cross section maximum. The ordinate of fig. 1 was calibrated by normalization of the high energy part in fig. 1 to the respective data in ref. [4]. These data were inserted in fig. 1 as a smooth curve. In comparison with the present data they demonstrate the effect of the decreased bandwidth of the exciting radiation:

The ionization threshold is more pronounced.

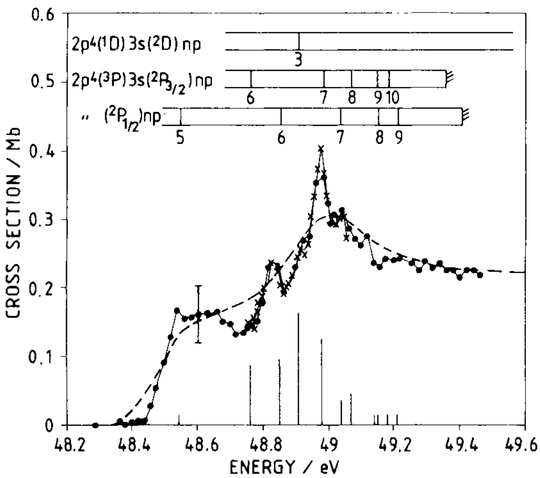

Fig. 1. Photoionization cross section for the Ne 2s-electron as function of the exciting photon energy. Statistical uncertainty in the order of the dot size. (——) Present data, (– – –) from ref. [4], vertical solid lines indicate positions and relative heights of resonances in arbitrary units from ref. [7].

It is followed by a short energy range of constant cross section values.

The single broad peak observed earlier splits up into a complicated structure with minima and maxima.

For Ar [3] and for Kr [5], structures in the energy dependence of the photoionization cross section could be correlated with structures in the total absorption cross sections [10,11]. The peaks observed in absorption for Ne [7,8] were inserted in fig. 1 as solid vertical lines with an uncertainty of 20 meV of their energy positions, resulting mainly from the fixing of the threshold in the experimental curve. They can be characterized by narrow absorption profiles and were identified as belonging to the $2p^4(^3P)$-$3s(^2P_{1/2,3/2})np$ series and to the $2p^4(^1D)3s(^2D)3p$ state. The relative strength of the absorption resonances taken from ref. [7] is given by the height of the vertical solid lines.

Figure 1 manifests unambiguously that the mentioned doubly excited states of the neon atom are responsible for the complicated energy dependence of the 2s-electron photoionization cross section near threshold. But it is also evident that more measurements with further reduced bandwidth of the exciting radiation are necessary for an identification of the influence of the single states. The intensity distribution of the resonances observed in photoabsorption and in the present experiment clearly differ from each other. The reason for this difference is probably the 2p-electron ionization channel which should also be influenced by the doubly excited atomic states. As a consequence, a complicated interference structure in both sub-valence shell ionization cross sections will result. Nevertheless the presented scan allows to conclude that a bandwidth of 40 meV should be sufficient for the determination of the cross section at the threshold. A threshold value of 0.17 Mb was measured with an accuracy of 25%, which is related to the accuracy of the value used for normalization [4]. The uncertainty of the latter depends on the error of the recommended 2s-electron photoionization cross sections [12]. The measured value of 0.17 Mb can be compared with 0.25 and 0.21 Mb, calculated at threshold by application of the random phase approximation RPAE [13] and the R-matrix method [14], respectively. The latter value is still within the experimental error bars while the RPAE value is too large.

In summary, a 40 meV bandwidth threshold scan of the 2s-electron photoionization cross section revealed for the first time details of a complicated structure resulting from the influence of a number of doubly excited atomic states. Further experiments with an even more reduced bandwidth of the exciting radiation and with an independent and accurate determination of the absolute threshold cross section will be of interest.

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