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Vanishing postcollision interaction in inner-shell photoionization

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When the photoelectron becomes faster than the Auger electron in a photoionization event the postcollision interaction should vanish. This vanishing effect has been investigated and confirmed in terms of both the absolute energies and line shapes for the N_5 -O₂₃O₂₃¹S₀ Auger electrons from xenon.

Since the first experimental investigations of postcollision interaction (PCI) in inner-shell ionization processes $1-3$ it has been realized that PCI is a phenomenon common to all inner-shell ionization processes close to threshold. The most obvious PCI phenomenon is the energy exchange between the fast Auger electron following the inner-shell ionization process and the slow ionized electron.⁴ In the present paper we concentrate on the most ideal case for PCI studies, i.e., the ejection of an Auger electron following photoionization with photon energies close to threshold. This process is simpler than the case of electron impact ionization. In the latter case, in particular, even at very high impact energies PCI will never vanish due to there always being a finite probability that a slow particle will be present in the final state.⁵

Experimental studies of PCI effects in inner-shell pho-Experimental studies of PCI effects in inner-shell photoionization⁶⁻¹³ have mostly concentrated on establishing the energy gain ϵ of the Auger electrons close to threshold and then comparing these energy shifts ϵ (and in a few cases also line shapes) with theoretical predictions. Fair agreement has been achieved so far, but there has been some criticism¹⁰ of the quantitative comparisons.

Since the first theoretical treatment of PCI in inner-shell photoionization processes by Niehaus¹⁴ a number of more advanced models have appeared in the literature. Of particular interest for the present paper are the most recent improvements of the Niehaus model as given by Helenelund et al., ¹⁵ Niehaus and Zwakhals, ¹⁶ and Russek and et al.,¹⁵ Niehaus and Zwakhals,¹⁶ and Russek and
Mehlhorn.¹⁷ These semiclassical models allow easy calcula tions of the PCI energy distribution; the only quantummechanical calculation for the special case considered in this Rapid Communication is that of Kuchiev and Sheinerman.¹⁸ But only the theory of Russek and Mehlhorn has been extended to take into account the time it takes for the fast Auger electron to overtake the slow photoelectron (compare also with Refs. 8 and 19). This has important consequences for the PCI effect as manifested in a different energy shift ϵ and, in addition, in a different line shape. In particular, within the classical picture, the PCI phenomenon should vanish for photon energies such that the photoelectron is faster than the Auger electron (the excess energy E_{exc} becomes larger than the kinetic energy E_A of the Auger electron). We will call this the no-passing effect.

It is the aim of this Rapid Communication to study experimentally the predictions of recent semiclassical PCI theories and, in particular, to investigate the no-passing effect. The experimental verification of this no-passing effect is of general interest to the further development of PCI theories (especially for electron impact ionization) and it is of fundamental importance for all determinations of inner-shell binding energies: It provides the simple but important criterion that for an excess energy E_{exc} larger than the kinetic energy E_A of the Auger electrons the PCI effect no longer plays a role in inner-shell photoionization processes.

For the present investigation we have chosen the case of $4d_{5/2}$ photoionization in xenon and the associated N₅-O₂₃O₂₃ ${}^{1}S_{0}$ Auger decay. The verification of the no-passing effect is based on two experimental subjects: on the absolute kinetic energies of Auger electrons and photoelectrons and on the line shape of the N_5 -O₂₃O₂₃¹S₀ Auger electrons.

The experiment was performed at the Berlin electron storage ring BESSY using a toroidal grating monochromator (TGM4). Of relevance to the success of our PCI investigation are the high photon flux and the small contribution of higher orders in the monochromatized light (for photon energies above 70 eV less than 0.5% in second order and a negligible amount in higher orders). Photoelectrons and Auger electrons from the interaction region of the photons with the target atoms were analyzed with a rotatable double-sector cylindrical mirror analyzer and, in addition, by a fixed monitor analyzer. Details for this experimental setup are given by Derenbach and Schmidt.²⁰ The energy resolution of the electron analyzer was approximately 0.7%, and the band pass of the monochromator varied from 0.2 eV at 68 eV to 0.9 eV at 125 eV. Accurate calibration of the electron kinetic energies required the introduction of helium into the interaction region in addition to the xenon target. The helium and xenon pressures in the source volume were 6×10^{-4} and 7×10^{-5} Torr, respectively, with a tank pressure lower by a factor of 10 (the background vacuum is 8×10^{-7} Torr).

First we discuss the influence of the no-passing effect on kinetic energies. Figure 1 shows the results for the kinetic energy E_A of the N₅-O₂₃O₂₃¹S₀ Auger line as function of the photon energy, together with theoretical data. The values cover the range from close to threshold, $E_{\text{exc}} = h\nu - E_B(4d_{5/2}) = 0.30$ eV, to the upper limit of the $E_{\text{exc}} - n\nu - E_B (+a_{5/2}) - 0.50$ ev, to the upper limit of the
monochromator ($h\nu \approx 124$ eV), $E_{\text{exc}} = 56.73$ eV. These experimental data suggest that for photon energies greater than 100 eV a constant value $E_{\rm A}^0$ = 29.97 \pm 0.02 eV is achieved.

A corresponding discussion can be made for the kinetic energy E_{ph} of the $4d_{5/2}$ photopeak. However, here two complications arise: On the one hand, this photopeak contains PCI effects in a more complicated manner resulting from the several distinct Auger decays which are possible. On the other hand, this photopeak is disturbed at low kinetic energy by a reduction in the transmission of the electron analyzer (instrumental cut-off effect). To avoid these effects only measurements for photon energies greater than

FIG. 1. Absolute kinetic energy E_A of the N₅-O₂₃O₂₃¹S₀ Auger line of xenon as a function of photon energy. Experimental data: \times (from both sectors of the electron energy analyzer). Theoretical predictions: no-passing effected included, -- (Russek and Mehlhorn, Ref. 17); no-passing effect neglected, $\frac{1}{2} \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \left(\frac{1}{2} \right)$ (Helenelund et al., Ref. 15); $-\cdot - \cdot$ [earlier Niehaus (Ref. 14) model].

100 eV, where $E_{\text{exc}} > E_A$ and PCI effects are expected to vanish, are examined here. These data show that in the region above 100-eV photon energy the value of $E_B(4d_{5/2})$ determined from $E_B(4d_{5/2}) = h\nu - E_{\text{ph}}^0$ is constant and equal to 67.55 ± 0.02 eV.

These constant values for both E_A^0 and E_B for photon energies above 100 eV provide our first experimental verification of the no-passing effect.

Our absolute values E_A^0 and E_B can be compared with data from the literature. This is of special interest because both the ionization potential of XeII and the ${}^{1}S_{0}$ energy level of the $5p⁴$ electron configuration in XeIII given in the Moore's²¹ tables have been revised. The critical analysis of Hansen and Persson²² provides highly recommended values for E_A^0 and E_B : E_A^0 = 29.967 ± 0.012 eV, E_B = 67.548 ± 0.011 eV (see also Ref. 23). The values obtained for E_A^0 and E_B in the present work are in perfect agreement with these data. This seems at a first glance quite surprising; the recommended E_B value comes from energy-loss spectrometry using 1.5-keV electron impact.²⁴ However, in this case of electron impact excitation also possible PCI effects must vanish.

Our verification of the no-passing effect in the region of $E_{\rm exc} > E_A$ is supported indirectly by the magnitude of relative energy shifts of the N_5 -O₂₃O₂₃¹S₀ Auger line in xenon for $E_{\text{exc}} < E_A$. This is demonstrated in Fig. 1 by comparing the experimental Auger energies with theoretical predictions. Of relevance to our discussion are the solid curve from the Russek and Mehlhorn¹⁷ model, which takes into account the no-passing effect, and the dashed curve from the model of Helenelund et al.,¹⁵ which neglects the nopassing effect (the model of Niehaus and Zwakhals¹⁶ gives results for neglected angular momentum exchange equivalent to those of Helenelund et al.;¹⁵ the quantummechanical approach of Kuchiev and Sheinerman¹⁸ does not consider the no-passing effect, for lower excess energies it agrees with the results from Helenelund et al., ¹⁵ and for $E_{\text{exc}} \geq E_A$ it predicts even larger energy shifts than Helenlund et al.¹⁵). We have checked at specific values of E_{exc} that both curves are identical if the no-passing effect is eliminated in the model of Russek and Mehlhorn. The chain curve from the earlier Niehaus¹⁴ model is also shown for convenience. It should be noted that all the theoretical curves are calculated for the same $4d_{5/2}$ -hole level width $\Gamma = 110$ meV,¹⁰ that they all have the same energy offset E_A^0 as reference for $E_{\text{exc}} \rightarrow \infty$, and that they all contain the influence of the instrumental resolution by folding the theoretical PCI distribution with the known spectrometer function. The influence of the spectrometer function on the observed energy shift has been discussed earlier.¹⁰ Here it varies between 0 and 40 meV depending on the model as well as on the excess energy. The comparison between the experimental data and the theoretical curves in Fig. 1 clearly demonstrates the no-passing effect on the energy shift in the region of small excess energies.

At this point a remark should be made concerning earlier

FIG. 2. Line shape of the N₅-O₂₃O₂₃¹S₀ Auger line of xenon. Experimental data (points with error bars) and theoretical predictions: no-passing effect included, — (Russek and Mehlhorn, Ref. 17); no-passing effect neglected, $- -$ (Helenelund et al., Ref. 15).

determinations¹⁰ of the relative energy shifts of this Auger peak. In those studies only relative energy shifts ϵ could be measured with $\epsilon = E_A - E_A$ ($E_{\text{exc}} = 42.45$ eV). With the information from the present investigation, $E_A(E_{\text{exc}}=42.45)$ eV) = E_A^0 , the relative shift ϵ can be placed on the absolute E_A scale and gives excellent agreement with the data of Fig. 1.

Our second experimental confirmation of the no-passing effect in the xenon N_5 -O₂₃O₂₃¹S₀ Auger spectrum is based on the observed line shapes. Such a critical test was feasible in the present experiment because the relevant photon energy range was free of contributions from higher orders. Figure 2 gives a selection of experimental line profiles taken at different photon energies together with two different theoretical curves; the solid curve is from the Russek and Mehlhorn¹⁷ model, the dashed curve from that of Helenelund et al .¹⁵ Here again the influence of the experimental spectrometer function on the theoretical PCI energy distribution has been taken into account. To compare the line shapes, the theoretical distributions are shifted such that their maxima coincide with the peak positions of the

- ¹M. J. van der Wiel, G. R. Wight, and R. R. Tol, J. Phys. B 9, L5 (1976).
- ²S. Ohtani, H. Nishimura, H. Suzuki, and K. Wakiya, Phys. Rev. Lett. 36, 863 (1976).
- 3V. Schmidt, N. Sandner, W. Mehlhorn, M. Y. Adam, and F. Wuilleumier, Phys. Rev. Lett. 38, 63 (1977).
- 4V. Schmidt, in X-Ray and Atomic Inner-Shell Physics, edited by B. Crasemann, AIP Conf. Proc. No. 94 (AIP, New York, 1982), p. 544.
- sW. Sandner (private communication).
- ⁶H. Hanashiro, Y. Suzuki, T. Sasaki, A. Mikuni, T. Takayanagi, K. Wakiya, H. Suzuki, A. Darjo, T. Hino, and S. Ohtani, J. Phys. B 12, L775 (1979).
- $⁷M$. K. Bahl, R. L. Watson, and K. J. Irgollic, Phys. Rev. Lett. 42,</sup> 165 (1979).
- ⁸T. C. Chiang, D. E. Eastman, F. J. Himpsel, G. Kaindl, and M. Aono, Phys. Rev. Lett. 45, 1846 (1980).
- ⁹G. S. Brown, M. H. Chen, B. Crasemann, and G. E. Ice, Phys. Rev. Lett. 45, 1937 (1980).
- ¹⁰V. Schmidt, S. Krummacher, F. Wuilleumier, and P. Dhez, Phys. Rev. A 24, 1803 (1981).
- ¹¹S. Southworth, U. Becker, C. M. Truesdale, P. H. Kobrin, D. W. Lindle, S. Owaki, and D. A. Shirley, Phys. Rev. A 28, 261 (1983).

experimental spectra (the correct position of the theoretical peak maxima are given in Fig. I). Figure ² clearly shows that the theoretical curve which includes the no-passing effect is also in very good agreement with the experimental line profile.

In contrast to this the shape of the PCI energy distribution without the no-passing effect deviates significantly from the experimental spectrum. For lower excess energies it is particularly the high-energy side of the PCI energy distribution which lies considerably above the experimental data. This is in accord with an earlier observation.¹⁰

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- ¹²K. Helenelund, S. Hedman, L. Asplund, U. Gelius, and K. Siegbahn, in Abstracts of Contributed Papers, International Conference on X-Ray and Inner-Shell Processes in Atoms, Molecules and Solids, Leipzig, 1984, edited by A. Meisel (unpublished), p. 184.
- 13G. B. Armen, T. Aberg, J. C. Levin, B. Crasemann, M. H. Chen, G. E. Ice, and G. S. Brown, Phys. Rev. Lett. 54, 1142 (1985).
- ¹⁴A. Niehaus, J. Phys. B 10, 1845 (1977).
- ¹⁵K. Helenelund, S. Hedman, L. Asplund, U. Gelius, and K. Siegbahn, Phys. Scr. 27, 245 (1983).
- '6A. Niehaus and C. J. Zwakhals, J. Phys. B 16, L135 (1983).
- ¹⁷A. Russek and W. Mehlhorn, J. Phys. B 19, 911 (1986).
- ¹⁸M. Yu. Kuchiev and S. A. Sheinerman, J. Phys. B 18, L551 (1985).
- '9G. N. Ogurtsov, J. Phys. B 16, L745 (1983).
- 20 H. Derenbach and V. Schmidt, J. Phys. B 17, 83 (1984).
- ²¹C. Moore, Atomic Energy Levels, Nat. Stand. Ref. Data Ser. Nat Bur. Stand. , No. 35, Vol. 3 (U.S. GPO, Washington, DC, 1971).
- 22J. E. Hansen and W. Persson, Phys, Scr. 25, 487 (1982),
- $23K$. Codling and R. P. Madden, Phys. Rev. Lett. 12, 106 (1964).
- 24G. C. King, M. Tronc, F. H. Read, and R. C. Bradford, J. Phys. B 10, 2479 (1977).