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Post-collision interaction in inner-shell ionization: The xenon case*

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The effect of post-collision interaction (PCI) in inner-shell ionization processes has been investigated observing the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectrum following ionization or excitation by photons with energies above (42 eV), close to (5.05, 0.85, 0.55, and 0.20 eV), and even below (− 0.05 eV) the $4d_{5/2}$ ionization threshold. A detailed quantitative analysis of the experimental spectra is given which takes into account the PCI energy shift and energy distribution as calculated in the semiclassical model of Niehaus. Good agreement between the experimental data and the theoretical predictions is achieved.

I. INTRODUCTION

When the transferred energy in the collision between a particle (electron, ion, photon) and an atom or molecule is close to the threshold for ejection of an inner-shell electron, the subsequent Auger decay may be influenced by the presence of the slow ejected electron (and possibly also by the slow scattered particle). This is a manifestation of the so-called post-collision interaction (PCI), an effect first studied in the decay of outer-shell autoionizing states following excitation by slow ion impact[1,2] or electron impact.[3] For further information about these PCI processes the reader is referred to the review articles by Read[4] and Niehaus.[5] Here we want to concentrate on PCI in inner-shell ionization processes which have found great interest in the last years experimentally (electron impact[6-9]; photon or quasiphoton impact[10-17]) as well as theoretically.[18-25] These PCI phenomena can be interpreted as a relaxation process (the slow electron from the ionization process suddenly moves in a changed potential when the fast Auger electron is ejected) or as a shielding effect (the slow electron partially screens the ionic field and therefore the ejected faster Auger electron sees a smaller attractive potential), i.e., PCI is a final-state correlation effect. It leads to an energy loss for the slow electron from the ionization process balanced by an equal gain in energy for the fast Auger electron. Experimentally, this is seen as a shift and broadening of the corresponding lines in the electron spectrum. An important quantity for PCI is the excess energy E_1^0, which is the difference between the energy of the incident particle or photon and the ionization energy of the atom. When the inner-shell ionization is caused by electron impact then there are two slow continuum electrons (energies E' and E'') with which the Auger electron can interact. Therefore the net PCI effect will depend also on the probability distribution of sharing the total excess energy $E_1^0 = E' + E''$ between the two slow electrons (see, for example, Ref. 26). This complicates a theoretical prediction of the PCI effect in electron-impact ionization considerably. A more direct case for the investigation of PCI in inner-shell ionization is given when the ionization is caused by photon impact since only one slow and one fast electron (photoelectron and Auger electron, respectively) can be subject to PCI. In this paper we report on PCI in the photoexcited xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger process. With respect to our earlier experimental investigations[13,14] our new electron spectra are of considerably improved quality (better statistics, smaller monochromator bandpass, spectra above and below the ionization threshold). This allows us to obtain more precise results and a more quantitative discussion of these results.

II. THEORETICAL CONSIDERATIONS

Before going into a detailed discussion of the PCI effect in the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectrum, let us first consider from a more general point of view how the electron spectrum is influenced when the photon energy is lowered towards and below the ionization threshold (compare Ref. 23). This is demonstrated schematically in Fig. 1 using the excess energy E_1^0 as a parameter. At high photon energy ($E_1^0 \gg 0$) the $4d$, $5s$, and $5p$ photoelectron peaks with their satellite lines[27-30] are well separated from the Auger lines (only one Auger line is shown in the figure for simplicity). For photon energies just above the $4d$ ionization threshold ($E_1^0 \geqslant 0$) PCI occurs and it shows up in energy gains ϵ for the Auger electron and energy losses $-\epsilon$ for the photoelectron. When ϵ exceeds E_1^0, i.e., $E_1^0 - \epsilon < 0$ then the pho-

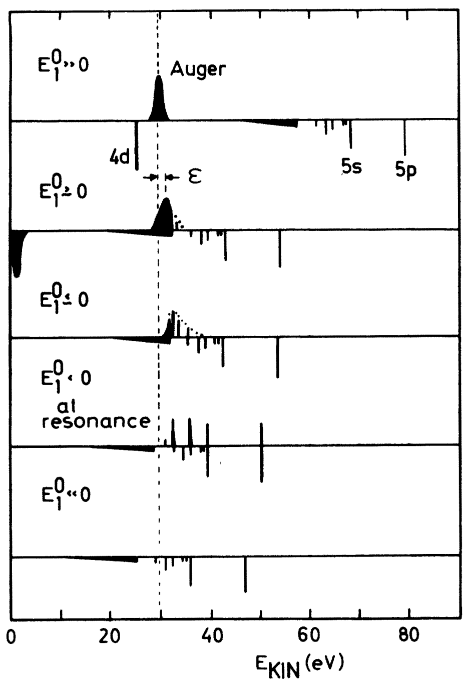

FIG. 1. Schematical representation of the electron spectrum following photoionization in xenon. The photoelectron spectrum ($5s$, $5p$, and $4d$ photopeaks are symbolized) is shown pointing downwards and the spectrum of Auger electrons (only one line is shown for simplicity) following the ionization of a $4d$ electron is shown pointing upwards. E_1^0 is the excess energy (photon energy minus threshold energy). For further explanation see text.

toelectron is "shaken down"[31] to a Rydberg orbital ($E_n < 0$) causing a discrete structure at higher kinetic energy with respect to the former Auger peak. These discrete lines can correspond to the same final-state configuration as the satellite lines resulting from ionization and simultaneous excitation of electrons from the $n = 5$ shell. The processes leading to these final states are undistinguishable and therefore interference effects are possible. For $E_1^0 < 0$ but still close to the threshold, $4d$ ionization is not possible and the former Auger peak has disappeared. However, excitation of a $4d$ electron to accessible high Rydberg states and subsequent autoionizing decay will produce final ionic states in the neighborhood of the former Auger peak which again interfere with the outer-shell satellite lines. The sudden transformation of the $4d$ hole into two outer-shell holes during the autoionizing decay can also be considered as a relaxation process. This mechanism and the dense series of high Rydberg states make the smooth shape of the Auger line intensity (see dotted line in Fig. 1 with E_1^0 around zero) observed for photon energies just around the inner-shell ionization threshold understandable. When the photon energy is lowered further, $4d$ excitation can occur only to well isolated resonance states[32,33] whose decay produces the spectrum of autoionized electrons.[34-37] Interference with photoelectron lines of outer-shell ionization processes is possible again and can show a drastic change of intensity in the outer-shell photoelectron spectrum when the photon energy is scanned across the inner-shell resonance (this has also been observed in a similar investigation on barium[38]). Finally, when no resonance excitation is possible ($E_1^0 \ll 0$) the undisturbed photoelectron spectrum of outer-shell ionization processes is observed.

In this work we want to concentrate on those processes with E_1^0 positive or slightly negative, i.e., processes above and just below threshold. The corresponding theory for inner-shell photoionization processes with subsequent Auger emission has been developed first by Niehaus.[18] It is a semiclassical description for PCI based on the Born-Oppenheimer separation of the motion of the slow electron from the motion of the other electrons. When only one initial and one final state is considered for simplicity, the results of the theory by Niehaus are equivalent to those of the classical model of Barker and Berry[2] taking into account the differences in the potentials for the slowly receding photoelectron, and they are also equivalent to those of the shake-down model of King *et al.*[31] transforming the transition amplitude of the Niehaus model from the time scale to that of the distance r of the photoelectron from its origin. Assuming for the potential energy curves of the singly and doubly ionized atom a Coulomb curve with $Z = -1$ or $Z = -2$, respectively,[39] the model of Niehaus provides an analytic expression for the energy distribution $P(\epsilon)$ of the energy gain ϵ of the Auger electron (energy loss $-\epsilon$ for the photoelectron). This distribution depends on the excess energy E_1^0 and the lifetime τ (alternatively level width Γ) of the inner-shell hole. This means that for a known value E_1^0 the PCI energy distribution should depend on only one parameter, namely Γ. From this energy distribution, the most probable energy shift ϵ^p can be determined as the position of the maximum, and the shake-down probability P_s as the ratio of the area with $\epsilon > E_1^0$ with respect to the total area of the distribution curve. Contrary to the case of two slow electrons in the continuum (see, for example, Ref. 40) little is known about the angular correlation between the slow photoelectron and fast Auger electron and about the threshold behavior of the cross section.[20] There are theories[19-22,24,25] more refined than the model of Niehaus. However, these more appropriate formulations do not provide for a simple analytic expression for the PCI energy distribution $P(\epsilon)$. They require more elaborate calculations which are not yet available for the case under consideration. Therefore, in order to make a quantitative analysis of the PCI effect in our xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectrum, the model of Niehaus shall be applied. In this case, some remarks shall be made.

(i) For $E_1^0 \rightarrow \infty$ the theoretical expression for the energy distribution $P(\epsilon)$ does not converge to a Lorentzian shape $L(\epsilon)$ for the Auger electrons and photoelectrons, respectively, i.e., the energy distribution $P(\epsilon)$ is valid only in that region close at threshold where $\epsilon \geq \Gamma/2$.[21] In our xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectra close to threshold this condition is fulfilled. Furthermore, small modifications in $P(\epsilon)$ will not show after convolution with the spectrometer function which in our case has a full width at half maximum (FWHM) of about 270 meV compared to a level width Γ of about 100 meV.

(ii) As has been demonstrated[18,20,41,42] interference structures due to PCI can occur in the electron spectrum. Necessary conditions for one kind of interference are coherent excitation of the initial states (compare also the PCI Stark mixing of the initial states[43]) and the same energy (due to PCI) of Auger electrons originating from different initial but same final ionic state of the Auger process. In the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectrum the same final states of the Auger process are separated by 2 eV because of the spin-orbit splitting in the $N_{4,5}$ shell, i.e., interference effects are not possible for $\epsilon \leq 2$ eV. Because nearly all possible energy shifts are smaller than this value these interference effects are neglected. Of course, the type of interference effects between Auger transitions with shakedown due to PCI and direct photoionization of satellite lines discussed above and with a background amplitude are still possible.

(iii) In the models cited above the energy distribution $P(\epsilon)$ depends (for given excess energy E_1^0) only on the half-width Γ or lifetime τ of the inner-shell hole. This lifetime has been taken to be constant thus neglecting the possible influence from the presence of the slow photoelectron.[33,43] One way to correct for this influence is to consider the lifetime as a free parameter in the calculation of $P(\epsilon)$.[44]

(iv) The energy distribution $P(\epsilon)$ in the model of Niehaus has been derived with the assumption of pure Coulomb character of the ionic potentials before and after the Auger transition. This is a good approximation for the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectra with $E_1^0 \geq 0.2$ eV because there the Auger transition occurs when the photoelectron is far away from the ion; however, for $E_1^0 = -0.05$ eV deviations might occur.

(v) For large values of ϵ (dominant shakedown processes and excitation of high Rydberg states) a quantum-mechanical description of the PCI effect according to the more refined theories cited above should be applied. However, the results of the classical theory are expected to be still qualitatively correct.[18]

III. EXPERIMENTAL DETAILS AND DATA ANALYSIS

The experiments were carried out using the synchrotron radiation from the Anneau de Collisions d' Orsay (ACO) storage ring. Two different types of monochromators were employed, one based on a Rowland circle mounting (RCM)[45] and one based on a holographic toroidal grating mounting (TGM).[46,47] The first investigations on PCI in inner-shell photoionization included investigation of disturbances due to second-order and stray light, the structure of the outer-shell photoelectron spectrum including the satellites, the resolution and contact potential of the electron analyzer, and the stability against instrumental energy shifts; these data have been obtained using the RCM.[13,14] The use of the TGM brought much higher photon flux over a long period of time which is due mainly to the ultrahigh-vacuum condition (10^{-9}-Torr range) that this monochromator is operating with (further details in Ref. 48). This enabled us to work with considerably reduced monochromator bandpass (about 6 times smaller) and, at the same time, to gain about two orders of magnitude in the counting rate. In this work, spectra have been taken at the following photon energies (uncertainty ±50 meV) with bandpass (BP): 110 eV, BP = 0.77 eV; 72.6 eV, BP = 0.15 eV; 68.4 eV, BP = 0.13 eV; 68.1 eV, BP = 0.13 eV; 67.75 eV, BP = 0.13 eV; 67.5 eV, BP = 0.13 eV. For comparison, the binding energy of a $4d_{5/2}$ or $4d_{3/2}$ electron in xenon is 67.548 or 69.537 eV, respectively.[33]

Xenon was used as the target gas at a pressure of about 1×10^{-4} Torr. Electrons ejected at a mean angle of 54°44′ with respect to the photon beam direction were accepted and analyzed by a cylindrical mirror spectrometer[35,49,50] with an instrumental resolution of 0.9%. From the N_5-$O_{2,3}O_{2,3}\ {}^1S_0$ Auger peak in the spectrum at 110-eV photon energy, the spectrometer function at 29.93-eV kinetic energy has been deduced fitting to the experimental data the result from an estimated spectrometer function folded with a Lorentzian distribution with $\Gamma = 100$ meV.[51,52] This spectrometer function then has been used as a standard for other kinetic energies E_{kin} taking into account the change of half-width ΔE based on the relation $\Delta E = 0.009E_{kin}$.

In order to probe instrumental shifts possibly disturbing the true PCI energy distributions of the threshold Auger spectra, the same procedure as in our former work[13,14] was used: the xenon Auger spectra were framed by measurements of the decay electrons of the $2s2p\ ^1P_1$ autoionizing state in helium using zero-order light from the monochromator. This investigation (with improved channel width) gave a reproducibility of better than ±18 meV. Second-order light from the monochromator and stray light disturb the Auger spectrum close to threshold in the same way. Below the N_4 threshold their net effect can be seen in the presence of the N_4-$O_{2,3}O_{2,3}\ ^1S_0$ Auger peak which makes the correction for this disturbance possible.

In order to obtain quantitative information on the PCI effect from the experimental spectra the following fitting procedure has been applied to the raw data. For the Auger spectrum at 110-eV photon energy the shape of one peak has been taken as the convolution of a Lorentzian distribution with the spectrometer function. The line positions were taken from the latest updated values available in the literature.[6,36,53] However, the line intensities given in Ref. 53 do not agree very well with the line intensities in our experimental spectrum, and therefore we have treated them as a free parameter in the fitting procedure. The result is shown as the solid line (including a straight-line background) in the corresponding part of Fig. 2, and Table I gives a compilation of the data and a comparison with the relative line intensities found by Werme *et al.*[53] for electron impact in the 4-keV energy range. The ratio of N_5-$O_{2,3}O_{2,3}$ to N_4-$O_{2,3}O_{2,3}$ Auger lines at 110-eV photon energy gives 1.50 in agreement with the branching ratio of the $4d_{5/2}$: $4d_{3/2}$ photolines at this energy.[54-56] At 72.6-eV photon energy and below, PCI effects occur in the Auger spectrum and the outer-shell photoelectron spectrum with its satellites and its double-ionization continuum moves into the region of the Auger spectrum. Furthermore, there is a contribution from stray

TABLE I. Kinetic energies and relative line intensities for the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger lines. Line identification is according to Hansen and Persson (Ref. 36), kinetic energies are from Werme *et al.* (Ref. 53), corrected by +0.2 eV according to Ohtani *et al.* (Ref. 6), relative intensity (a) is the present work for 110-eV photon energy, and relative intensity (b) is for 4-keV electron impact (Werme *et al.*).

Transition	E_{kin} (eV)	Relative intensity (%) (a)	(b)
N_5-$O_{2,3}O_{2,3}\ ^1S_0$	29.93	73	73
N_4-$O_{2,3}O_{2,3}\ ^1S_0$	31.91	102	100
N_5-$O_{2,3}O_{2,3}\ ^1D_2$	32.29	97	97
N_5-$O_{2,3}O_{2,3}\ ^3P_1$	33.19	37	39
N_5-$O_{2,3}O_{2,3}\ ^3P_0$	33.41	44	48
N_4-$O_{2,3}O_{2,3}\ ^1D_2$	34.27	71	104
N_5-$O_{2,3}O_{2,3}\ ^3P_2$	34.41	99	86
N_4-$O_{2,3}O_{2,3}\ ^3P_1$	35.19	46	43
N_4-$O_{2,3}O_{2,3}\ ^3P_2$	36.40	14	15

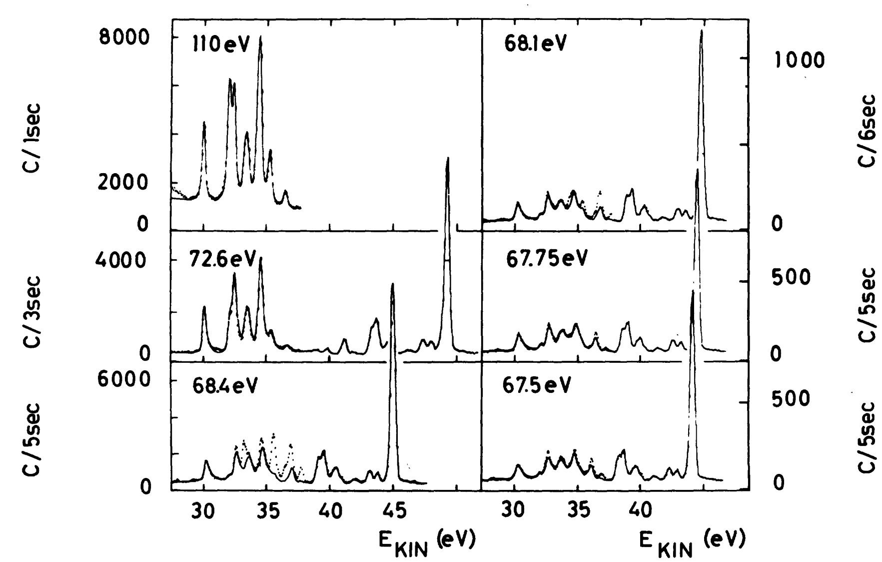

FIG. 2. Electron spectra of xenon following ionization by photons of distinct energies as given in the figure. Bars = experimental data, and solid line = total fit as described in the text.

light and higher orders diffracted from the grating and a constant background. Neglecting possible interference effects (compare above) the fitting procedure was applied assuming independent individual contributions. The Auger spectrum itself has been calculated folding the PCI energy distribution $P(\epsilon)$ as given by Niehaus[57] with the spectrometer function determined before. The resulting distributions $P_c(\epsilon)$ have been adapted in their relative intensities according to the values of Table I. At 72.6-eV photon energy a change between the N_5- and N_4-group intensity was allowed giving the branching ratio 2.45 which is in agreement with our former determination[56]; below 69.5-eV photon energy no N_4-$O_{2,3}O_{2,3}$ Auger spectrum is possible. Furthermore, the resulting distributions $P_c(\epsilon)$ have been shifted in energy in accord with the prediction of the PCI model. Hereby the PCI effect at 110-eV photon energy has been taken into account. In these calculations some properties of the convoluted PCI distribution $P_c(\epsilon)$ turned out to be important.

(i) $P_c(\epsilon)$ is very insensitive to the value chosen for E_a in the theory of Niehaus. E_a in a.u. is the reciprocal value of the radius of that atomic shell from which the photoelectron is ejected. Here a value $E_a = 1/0.87$ a.u. has been used.[58]

(ii) The shape of $P_c(\epsilon)$ changes only little with the value of Γ (about 100 meV) when Γ is varied within less than $\pm 20\%$, but the maximum position of $P_c(\epsilon)$ naturally depends on Γ.

(iii) The descending branch ($\epsilon \geq \epsilon^p$) of $P_c(\epsilon)$ was found to be always too high. This discrepancy is decreased by multiplying $P(\epsilon)$ with a factor f defined as $f = 1 - 0.1(\epsilon - \epsilon^p)/\epsilon^p$ when $f \geq 0$, otherwise it is set $f = 0$.

(iv) Because of the very asymmetric shape of the PCI energy distribution the most probable energy shift ϵ^p of the function $P(\epsilon)$ does not necessarily agree with that of $P_c(\epsilon)$, ϵ_c^p, which takes into account the influence of the spectrometer function.

The contribution of stray light and higher orders from the monochromator has been extracted from the raw experimental data themselves using the N_4-$O_{2,3}O_{2,3}$ $^1S_0$ Auger peak in the spectra below the N_4-ionization threshold as representative for these processes. The same correction weighted only with the measuring time has been applied to all spectra. The outer-shell photoelectron spectrum with its satellites and its double-ionization continuum has been determined in the region of the Auger lines by adapting the spectrum known at higher energies to those satellite lines which are still separated from the Auger lines (the slight change in the monochromator bandpass is negligible, but the influence of the spectrometer resolution has been taken into account). A straight-line background is also present in all spectra. Figure 3 shows, for example, the experimental spectrum from the N_5-$O_{2,3}O_{2,3}$ $^1S_0$ Auger peak to the 5s photoelectron peak at 67.75-eV photon energy together with the total fit and the individual fit contributions. Figure 2 gives the compilation of the experimental spectra and of the total fit. It should be noted that the total fit is based on the available information about the individual contributions which are handled equally for all experimental spectra and not on a possible best fit to each individual experimental spectrum.

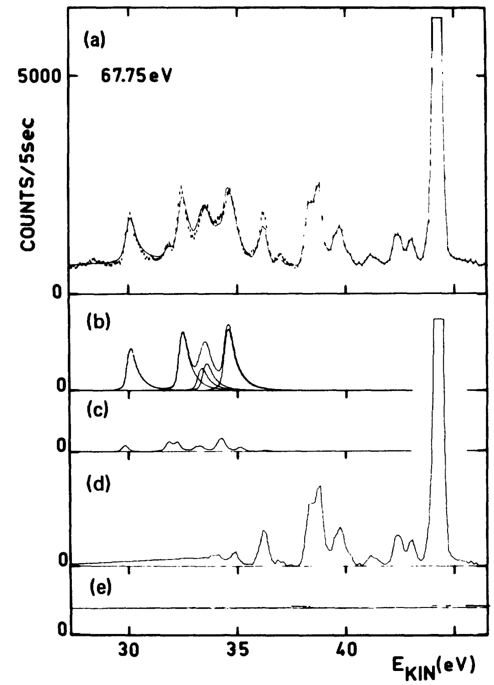

FIG. 3. Electron spectrum of xenon from the $N_5-O_{2,3}O_{2,3}$ $^1S_0$ Auger to the 5s photoelectron peak taken at 67.75 eV photon energy. a = experimental data (bars) and total fit (solid line); b = PCI Auger spectrum from $4d_{5/2}$ ionization with individual contributions; c = contribution from higher orders and stray light through the monochromator; d = contribution from 5s photoionization with satellites and double ionization; e = background.

IV. RESULTS AND DISCUSSION

Comparing the experimental data with the total fit of individual contributions to the electron spectrum between the N_5-$O_{2,3}O_{2,3}$ $^1S_0$ Auger peak and the 5s photoelectron peak (see Fig. 2), one notices a generally good agreement, except at 68.4-eV photon energy. This deviation can be explained as follows: At 68.4-eV photon energy the bandpass of 0.13 eV allows excitation of the $4d^95s^25p^6(^2D_{3/2})7p\ ^1P_1$ resonance at 68.34 eV which

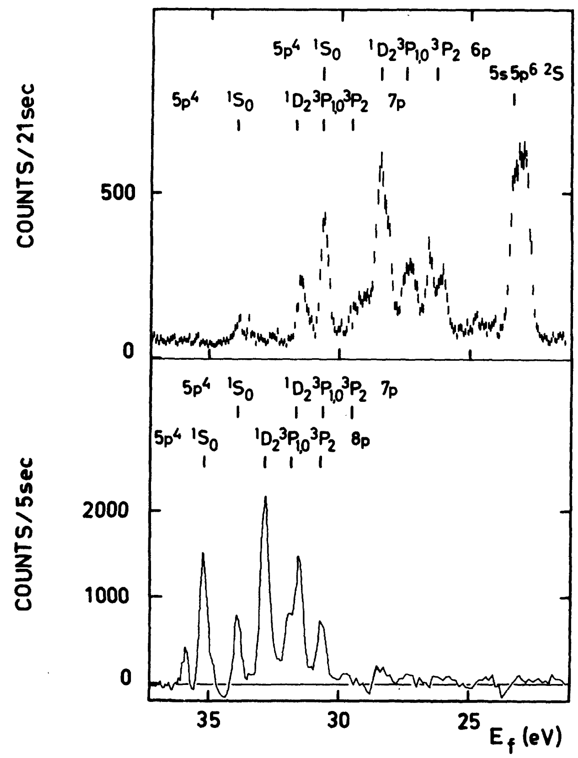

FIG. 4. Decay channels of $4d$ excitation resonances in xenon shown as function of the energy E_f of the final ionic state. Upper part [experimental data Ref. 35)]: $4d^9 5s^2 5p^6 (^2D_{5/2}) 6p\ ^1P_1$ resonance decay (with contributions from direct ionization); lower part (difference spectrum, this work; for more details, see text): $4d^9 5s^2 5p^6 (^2D_{3/2}) 7p\ ^1P_1$ resonance decay.

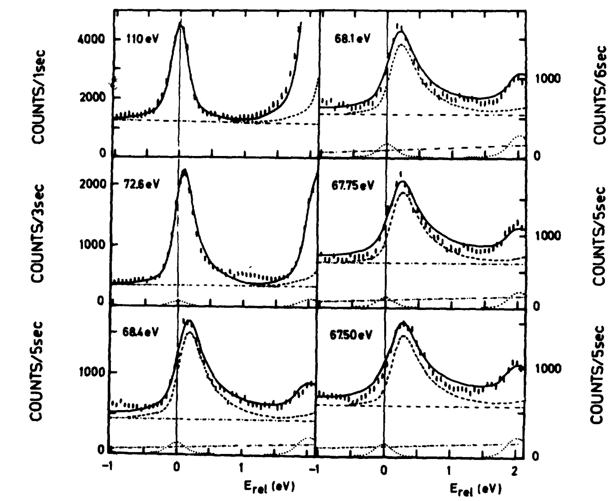

FIG. 5. Xenon $N_5 - O_{2,3}O_{2,3}\,^1S_0$ Auger peak following the ionization of a $4d_{5/2}$ electron ($E_B = 67.548$ eV) by photons of distinct energy as indicated in the figure. Bars = experimental data; —— = total fit; --- = Auger spectrum with PCI; -·-· = background; -··- = contribution from the double-photoionization continuum; ····· = Auger intensity (without PCI) due to stray light and higher orders from the monochromator.

has a half-width $\Gamma_r = 0.11$ eV.[32] When the 0.05-eV uncertainty in our photon energy is included the resonance can be covered nearly completely by the energy distribution of the monochromatized photons. The decay of this resonance then gives rise to additional lines in the electron spectrum (compare the case "$E_1^0 < 0$, at resonance" of Fig. 1). In principle, these lines can interfere with those following direct ionization in the outer shell. However, in a first approximation, one can neglect this possibility of interference effects and obtain a qualitative indication on the possible decay channels of this resonance from the difference between the experimental spectrum and the result of the fitting procedure as explained in the previous paragraph (i.e., accounting for all possible contributions except for the resonance decays). The result is shown in the lower part of Fig. 4. The assignment of these decay channels makes use of the analogy to the decay of the $4d^9 5s^2 5p^6 (^2D_{5/2}) 6p\,^1P_1$ resonance at 65.11 eV (Ref. 35; compare also Ref. 34). The decay channels of this resonance (together with the contribution from direct ionization) are shown in the upper part of Fig. 4, plotted for the same energies E_f of the final ionic state as in the lower part. The labeling is based on the rectified identification given in Ref. 36. The point of relevance here is that, in addition to the spectator transitions to $5p^4(^{2S+1}L_J)6p$, shake-up transitions to $5p^4(^{2S+1}L_J)7p$ also occur with remarkable intensity. In analogy to this result we can identify the spectator transitions of the $4d^9 5s^2 5p^6 (^2D_{3/2}) 7p\,^1P_1$ resonance to the $5p^4(^{2S+1}L_J)7p$ states and suggest the attribution of the remaining, unidentified lines to shake-up transitions to $8p$ states, as indicated in the figure. Three remarks should be made concerning the decay of the $4d^9 5s^2 5p^6 (^2D_{3/2}) 7p\,^1P_1$ resonance.

(i) The shake-up transitions to $8p$ seem to be even more intense than the spectator transitions; the reason for that is not yet understood.

(ii) The decay channels to $5s5p^6\,^2S$ and possibly other satellite lines of the outer-shell photoelectron spectrum are also possible but they do not show up in the difference spectrum plotted in the lower part of Fig. 4 because this region of the spectrum has been fitted to the experimental data.

(iii) This resonance decay could not be seen in the PCI experiment on xenon at 68.3-eV photon energy quoted in Ref. 14 because there the broad bandpass (BP = 1.6 eV) made the intensity of the resonance decay channels small with respect to that of the direct ionization process and therefore also to that of the subsequent Auger transitions.

TABLE II. Positions ϵ of the xenon N_5-$O_{2,3}O_{2,3}\,{}^1S_0$ Auger peak as function of the excess energy E_1^0. ϵ^p follows from the distribution $P(\epsilon)$ of the Niehaus (Ref. 18) model using $\Gamma=110$ meV, ϵ_c^p follows from the convoluted distribution $P_c(\epsilon)$, and $\tilde{\epsilon}_c^p$ relates ϵ_c^p to the shift at 110-eV photon energy. The experimental values of $\tilde{\epsilon}_c^p$ have an error of ±30 meV.

Excess energy (eV)	Peak positions (meV) Theoretical			Experimental
E_1^0	ϵ^p	ϵ_c^p	$\tilde{\epsilon}_c^p$	$\tilde{\epsilon}_c^p$
42.45	31	63	0	0
5.05	89	153	90	100
0.85	190	254	191	194
0.55	216	280	217	222
0.20	262	326	263	264
−0.05	305	369	306	294

Even though the total fit to the experimental data is not perfect, one can conclude that the main features of the experimental spectra obtained for all photon energies used in this work are understood on the basis of individual-fit contributions. This implies that the PCI effect in the xenon $N_{4,5}$-$O_{2,3}O_{2,3}$ Auger spectrum is described reasonably well by the semiclassical model of Niehaus slightly modified by the correction factor given above. In particular, it proves that the PCI energy distribution (shape of the former Auger peak) does indeed cross the threshold of inner-shell photoionization smoothly as was predicted by Niehaus and observed experimentally here for the first time. For a quantitative analysis of the effect of PCI we will now concentrate on the N_5-$O_{2,3}O_{2,3}\,{}^1S_0$ peak, as it is well separated from the rest of the spectrum and thus simplifies the discussion. Figure 5 therefore shows this peak on an enlarged scale together with the total-fit curve of Fig. 2 (solid line) and the individual contributions as discussed in Fig. 3. It shows the generally good agreement between the theoretical model and the experimental results. The small deviations between theory and experiment visible on this enlarged (and thus very sensitive) scale demonstrate the limits of the fitting procedure and ultimately of the theoretical model. However, a PCI quantity much simpler and easier to extract than the whole line shape is the position of the peak. This is presented in Table II for the investigated values of the excess energy E_1^0. Here, $\tilde{\epsilon}_c^p$ refers to the observed shift of the peak maximum with respect to the peak position at 110-eV photon energy. Figure 6 shows a plot of $\tilde{\epsilon}_c^p$ as a function of the excess energy E_1^0 together with our earlier experimental data[13,14] and compares them to theoretical predictions. The earlier experimental data provide less information because

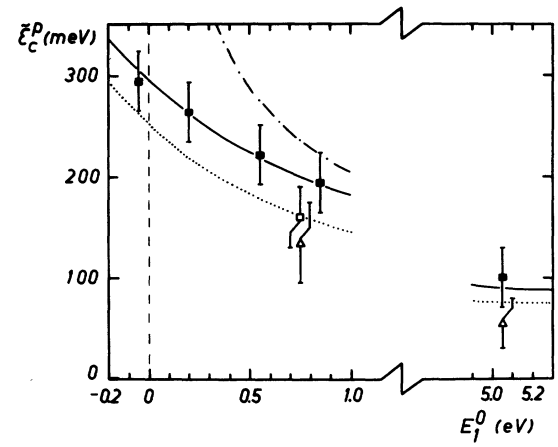

FIG. 6. Energy shift $\tilde{\epsilon}_c^p$ of the $N_5-O_{2,3}O_{2,3}\,{}^1S_0$ Auger peak (relative to its position at 110-eV photon energy) as function of the excess energy E_1^0. ■ = present work, △ = Schmidt *et al.* (Ref. 13), □ = Schmidt *et al.* (Ref. 14); —— and ······ = calculation according to Niehaus (Ref. 18) with Γ = 110 and 82 meV, respectively; —·— = calculation according to Barker and Berry (Ref. 2) with Γ = 110 meV.

of the much broader bandpass and stray-light problems (not considered in Ref. 13, probably underestimated in Ref. 14). Best agreement between experimental and theoretical values of $\tilde{\epsilon}_c^p$ based on the PCI model of Niehaus is given for $\Gamma=110$ meV (solid line). Using a value $\Gamma=82$ meV (Ref. 59) gives the dotted curve. The theoretical model which uses the half-width Γ of the inner-shell hole as the only adjustable parameter describes the energy shift very well over the energy region of this work. The value $\Gamma=110$ meV is compatible with the lifetimes of $4d$ excited states as quoted by Ederer and Manalis[32] but lower than the value of (129 ± 8) meV as suggested by King *et al.*[33] Whether this half-width Γ is equal to the half-width Γ_0, undisturbed by PCI, cannot be answered by this experiment. But it seems that the difference is smaller than in the investigation of the PCI effect in the argon $L_{2,3}$-$M_{2,3}M_{2,3}$ Auger spectrum (Hanashiro *et al.*[17] use $\Gamma=0.17$ eV, whereas Krause and Oliver[60] give $\Gamma_0=0.127$ eV). For a fixed value of Γ, the model of Niehaus predicts at higher excess energies E_1^0 the same energy shift as the model of Barker and Berry[2] which assumes a constant velocity of the slow electron which is not fulfilled for PCI in inner-shell ionization processes. The deviation starts towards lower values of E_1^0 where the most probable energy shift in the model of Barker and Berry goes to infinity at threshold (dash-dotted line in Fig. 6). This is altered in the theory adequate to inner-shell photoionization processes;

here $\mathcal{E}_c^p$ crosses the ionization threshold smoothly in accordance with our experimental results.

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