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# MEASUREMENT OF THE AUGER DECAY AFTER RESONANCE EXCITATION OF Xe 4d AND Kr 3d RESONANCE LINES

by



W. Eberhardt, G. Kalkoffen
*II. Institut für Experimentalphysik der Universität Hamburg*

and

C. Kunz
*Deutsches Elektronen-Synchrotron DESY, Hamburg*

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Measurement of the Auger decay after resonance excitation of Xe 4d and Kr 3d resonance lines

W. Eberhardt (a), G. Kalkoffen (a), and C. Kunz (b)

(a) II. Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-2000 Hamburg 50

(b) Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, D-2000 Hamburg 52

*The $N_{4,5}O_{2,3}O_{2,3}$ Auger spectra from Xe and the $M_{4,5}N_{2,3}N_{2,3}$ Auger spectra from Kr are investigated for different photon energies around threshold of ionization. When exciting at the resonance line ($4d^9 5s^2 5p^6 6p$ for Xe and $3d^9 4s^2 4p^6 5p$ for Kr) we observe the usual Auger multiplet structure to be shifted to higher kinetic energies. Additionally, new lines appear which can be assigned to shake-up processes in the $Xe^+$ and $Kr^+$ ions.*



## 1. Introduction

Auger spectra usually are obtained for excitation energies (photons or electrons) above threshold of ionization. The $N_{4,5}O_{2,3}O_{2,3}$ Auger spectrum of Xe and the $M_{4,5}N_{2,3}N_{2,3}$ Auger spectrum of Kr are analyzed in Ref. 1-3. Those spectra are rather independent of the excitation energy at photon energies way above threshold. When the excitation energy is lowered to a few eV above threshold post-collision interaction (PCI) effects due to a non-negligible coupling of the electron leaving the atom with the rest of the system are observed[3,4,5] An even stronger coupling occurs when the atom is excited to a resonance state below threshold. Such a state will decay either radiatively or via an Auger process which can be considered as a special type of autoionization.

We present here the first photoemission measurements of the Auger decay after excitation of Xe to the $4d^9 5s^2 5p^6 (^2D_{5/2}) 6p$ and to the $4d^9 5s^2 5p^6 (^2D_{3/2}) 6p$ resonance states at 65 eV and 67 eV respectively and after excitation of Kr to the $3d^9 4s^2 4p^6 (^2D_{5/2}) 5p$ and $3d^9 4s^2 4p^6 (^2D_{3/2}) 5p$ states at 91.2 eV and 92.4 eV respectively. Such investigations could not be carried out before the availability of a strong tunable light source like synchrotron radiation. They have considerable relevance for a detailed knowledge of the mechanism of deexcitation of certain resonance excitations and also towards a better understanding of correlation effects in excited atoms.

## 2. Experimental procedure

Synchrotron radiation from the storage ring DORIS was monochromatized by the grazing incidence monochromator FLIPPER[6]. The band pass of the monochromator was set at 0.3 eV. Xenon was used at a pressure of about $1 \times 10^{-4}$ Torr in a directed gas beam. The photoelectrons were analyzed with a commercial double pass cylindrical mirror analyzer at a cone with a $2\pi$ azimutal and a $12^o$ polar acceptance.

The axis of the cone was perpendicular to the direction of the photon beam and at 45° relative to the electric vector of polarization. These parameters are fairly unimportant for measurements of Auger lines. Especially the β-parameter, which is important for the observation of directly excited photoelectrons, has no relevance. The analyzer was used with a band pass of 0.3 eV. The counting rate was typically 30 pulses/sec in the Auger maxima.

## 3. Results

In Fig. 1 we show the absorption spectrum of Xe in the region of the onset of the 4d transitions. The resonance lines are superimposed onto a background of 5p and 5s electron excitations. Figure 1 serves as a reference for illustrating the different excitation processes we have used in the investigations of the Auger decay described as follows. The $N_{4,5}O_{2,3}O_{2,3}$ part of the whole Auger spectrum of Xe taken at 76.7 eV photon energy (an energy well above the ionization threshold for the 4d shell) is shown in Fig. 2a. There are two groups corresponding to transitions from vacancies in the $N_4$ and $N_5$ subshells. In view of the resonance excitation, only the peaks originating from a $N_5$ hole are labelled according to Othani et al.[3]. Figure 2b shows the Auger spectrum after excitation to the $4d^9 5s^2 5p^6(^2D_{5/2})6p$ resonance state at 65 eV. In analogy, Fig. 3 presents the $M_{4,5}N_{2,3}N_{2,3}$ part of the whole Auger spectrum of Kr taken at 117.5 eV photon energy and after excitation to the $3d^9 4s^2 4p^6(^2D_{5/2})5p$ resonance state at 91.2 eV. In addition to the Auger lines the spectra obtained with resonance excitation, show the Xe 5s and Kr 4s lines of the directly emitted photoelectrons.

## 4. Discussion

In the case of resonance excitation there is an overall shift to higher kinetic energies. This energy difference is mainly to be understood as an energy being gained from the increase in binding energy of the 6p electron for Xe and the 5p electron for Kr, due to the formation of a double vacancy in the 5p (Xe) and the



4p (Kr) subshells. The energies ($E_f$) of the different final states of the configurations Xe $4d^{10}5s^25p^46p$ and Kr $3d^{10}4s^24p^45p$ are obtained from Moore[7]. At the example of the $5s^25p^4(^1S)$ 6p state of $Xe^+$ we want to explain our considerations. An energy separation of 17.4 eV is obtained between the states $5s^25p^5(^2P_{3/2}) \rightarrow 5s^25p^4(^1S)6p$. Together with the ionization energy of a $5p_{3/2}$ electron in neutral Xe (12.1 eV) we obtain a total energy of 29.5 eV for the $5s^25p^4(^1S)6p$ final state. The kinetic energies $E_{kin}$ of the emitted electrons are given by the difference between the energy $E_i$ injected into the system and the energies $E_f$ of possible final state configurations. These are in our special case: $E_i = h\nu = 65$ eV for the resonance excitation from $4d^{10}5s^25p^6 \rightarrow 4d^9\ 5s^25p^6(^2D_{5/2})6p$ and $E_f = 29.5$ for producing the $5s^2\ 5p^4(^1S)6p$ configuration. The kinetic energy $E_{kin} = h\nu - E_f = 35.5$ eV for the $^1S$ peak falls at a 5.9 eV higher energy than the energy of the same peak when exciting far above threshold. (For the case of $Xe^{++}$ we obtain $E_{kin} = E_B - E_f = 29.6$ eV with the binding energy $E_B = 67.55$ eV[11] of a $4d_{5/2}$ electron and $E_f = 37.96$ eV[7] for producing the $5s^25p^4(^1S)$ configuration.) In analogy, we calculate an energy difference of about 4.4 eV for the $^3P$ peaks. The energy difference of about 1,5 eV between these values indicates the different coupling of the 6p electron to the $5s^25p^4$ core. The electron energies $E_{kin} = h\nu - E_f$ are indicated in Figs. 2,3 for the resonance excitation. The energies are in good agreement with observed maxima. In contrast to the case of excitation above threshold, only one series is involved because of our selective excitation of the $4d_{5/2}$ state of the hole in Xe ($3d_{5/2}$ for Kr). This makes the interpretation of the spectra easier.

In addition to these main Auger lines, which we could identify after Moore, new peaks (1-4 in Figs. 2,3) are observed. These peaks probably result from a shake-up process accompanying the Auger transition. A shake-up process is generally described as a transition between two states as the result of a sudden perturbation. It is a transition conserving parity (see e.g. Ref. 10). For the series $5s^25p^5np$ of $Xe^+$

we estimate an energy separation of 3.3 eV between the $5p^{4}6p$ and $5p^{4}7p$ states by taking the optical data[7] from the $5s^{2}5p^{5}6p$ and $5s^{2}5p^{5}7p$ states of Cs, since the energies of the $5s^{2}5p^{4}7p$ states of $Xe^{+}$ are not listed in Moore's tables[7]. A shift of the different states of the configurations $5s^{2}5p^{5}6p$ of $Xe^{+}$ by 3.3 eV leads to the positions marked 1-4 in Fig. 2b. In a similar way, we obtain an energy separation of the same order of magnitude between the $4s^{2}4p^{5}5p$ and $4s^{2}4p^{4}6p$ states of Kr using the data[7] for Rb (Fig. 3). In both cases the good coincidence with the measured spectrum supports the relevance of this interpretation. The shake-up processes apparently have a probability of the same order of magnitude as those without shake-up. Analogously Krause and Carlson[3] found that for Kr $M_{4,5}NN$ the double electron emission, as a special case of shake-up in the Auger process, competes strongly (≈30 %) with the single Auger process.

We also have measured the Auger spectrum after excitation to the second resonance state $4d^{9}5s^{2}5p^{6}(^{1}D_{5/2})7p$ at 66.3 eV for Xe (Fig. 2d). The marks in Fig. 2d indicate the kinetic energy of the electrons calculated by $E_{kin} = h\nu - E_f - \Delta E_{6p\rightarrow 7p}$ = 66.3 eV - $E_f$ - 3.3 eV, with the energy $E_f$ of the $5s^{2}5p^{5}6p$ final state configuration and the energy difference $\Delta E$ between the states $5s^{2}5p^{4}6p \rightarrow 5s^{2}5p^{4}7p$ as estimated before. The marks are in good agreement with the main structures. If we have no shake-down, the mean structures on the high kinetic energy side should correspond to Auger processes without shake-up retaining a $5s^{2}5p^{5}7p$ final state configuration. This also supports the assumption that after excitation to the first resonance line as discussed above the dominant structures besides the single Auger lines originate mainly from $5s^{2}5p^{4}6p \rightarrow 5s^{2}5p^{4}7p$ shake-up transitions. Contributions from shake-up to higher excited states, as for example 8p or 9p for Xe could not be identified.



The spectrum of Xe (Fig. 2c) taken at the energy for the 6p resonance excitation of the spin orbit partner of the electrons from the 4d shell, 67 eV for the excitation from the $N_4$ subshell, show nearly the identical structures of Fig. 2b with a 2 eV higher electron energy corresponding to the higher photon energy. Only the peak at about 38.5 eV in Fig. 2b which we cannot really explain at the moment doesn't appear in that spectrum.

An attempt to attribute any peaks to shake-up processes connected with the directly excited 5p or 5s electrons of Xe (4p,4s for Kr) is not justified, since we could show that these are by about one order of magnitude weaker. For proving this we have chosen an excitation energy between two resonance states of the 4d excitation, namely 65.8 eV between the 6p and 7p states of Xe (Fig. 1) and 92.8 eV for the 3d excitation of Kr. The cross section for the production of a d hole is practically zero there and therefore no Auger lines are observed. But of course, the 5s and 5p (4s,4p) lines of the direct excitation are excited with practically the same intensity as at the resonance energies. The amplitudes of the satellites are only about 10 % of the amplitudes of the Auger lines in the spectra Fig. 2,3.

## 5. Conlcusions

A source with tunable photon energy permits a selective excitation of the atomic shells. Using synchrotron radiation we were able to perform a detailed analysis of the mechanism of deexcitation of the Xe 4d and Kr 3d resonance excitations. After excitation to the 6p(Xe) and 5p(Kr) resonance line the usual Auger multiplet structure is generally shifted by the relaxation energy of about 5 eV for Xe and Kr to higher kinetic energies. We could also show that there is nearly the same probability for the two atoms to decay over the single Auger transition and over a Auger transition accompanied by a shake-up process leading to $5s^{2}5p^{4}7p$ and $4s^{2}4p^{4}6p$ excited states in Xe and Kr. The comparison between the measured spectra and the energies

obtained from optical data[7] demonstrates the relevance of core rearrangement and other correlation effects in Auger transitions.

## 6. Acknowledgement

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Figure Captions

Fig. 1 Cross ection versus photon energy for Xenon at the onset of the 4d electron excitation measured with a resolution of 0.04 eV. The indicated monochromator band pass of 0.3 eV shows the energy width used for the Auger measurements.

Fig. 2 NOO Auger spectra of Xe taken at different photon energies: above threshold of ionization of the 4d shell (a), at the energy for the 6p resonance excitation of the $4d_{5/2}$ shell (b), at the energy for the 6p resonance excitation of the $4d_{3/2}$ shell (c), at the energy for the 7p resonance excitation of the $4d_{5/2}$ shell (d). The peak labeled 5s is due to the direct ejection of electrons from the 5s shell.

Fig. 3 MNN Auger spectra of Kr at two different photon energies: above threshold of ionization of the 3d shell (a), at the energy for the 5p resonance excitation of the $3d_{5/2}$ shell (b). The peak labeled 4s is due to the direct ejection of electrons from the 4s shell.

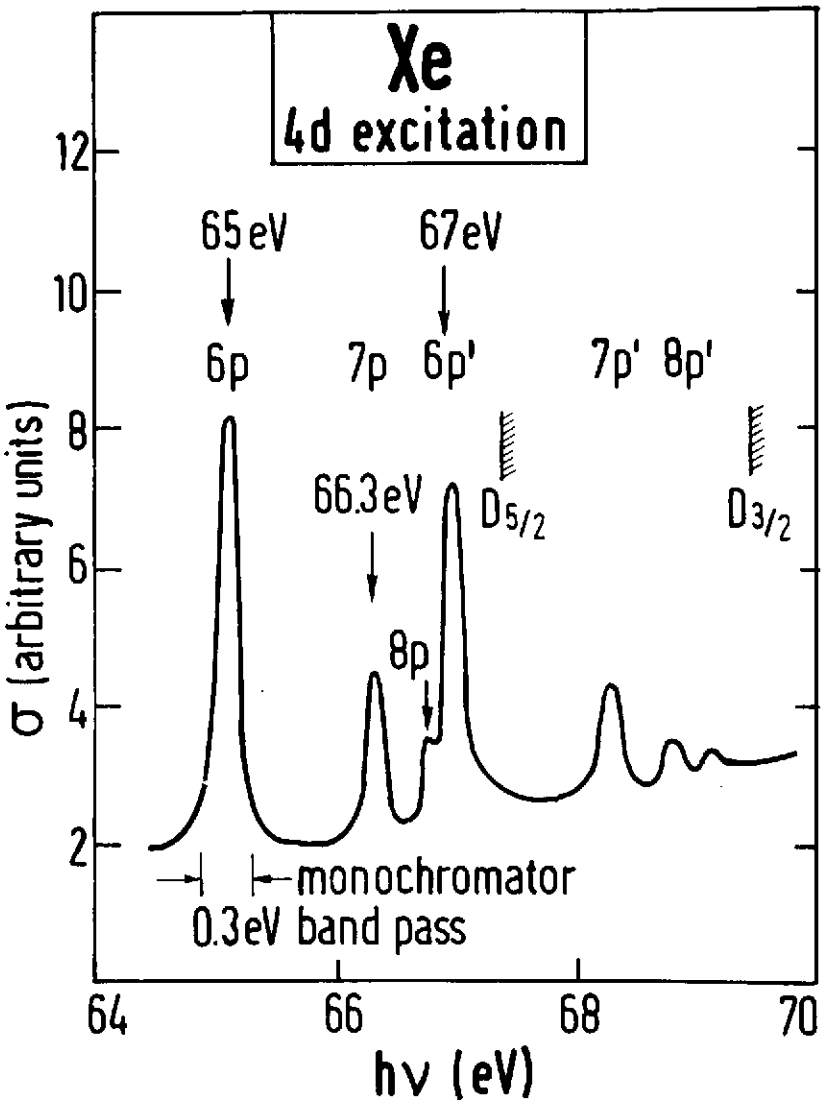


Fig. 1

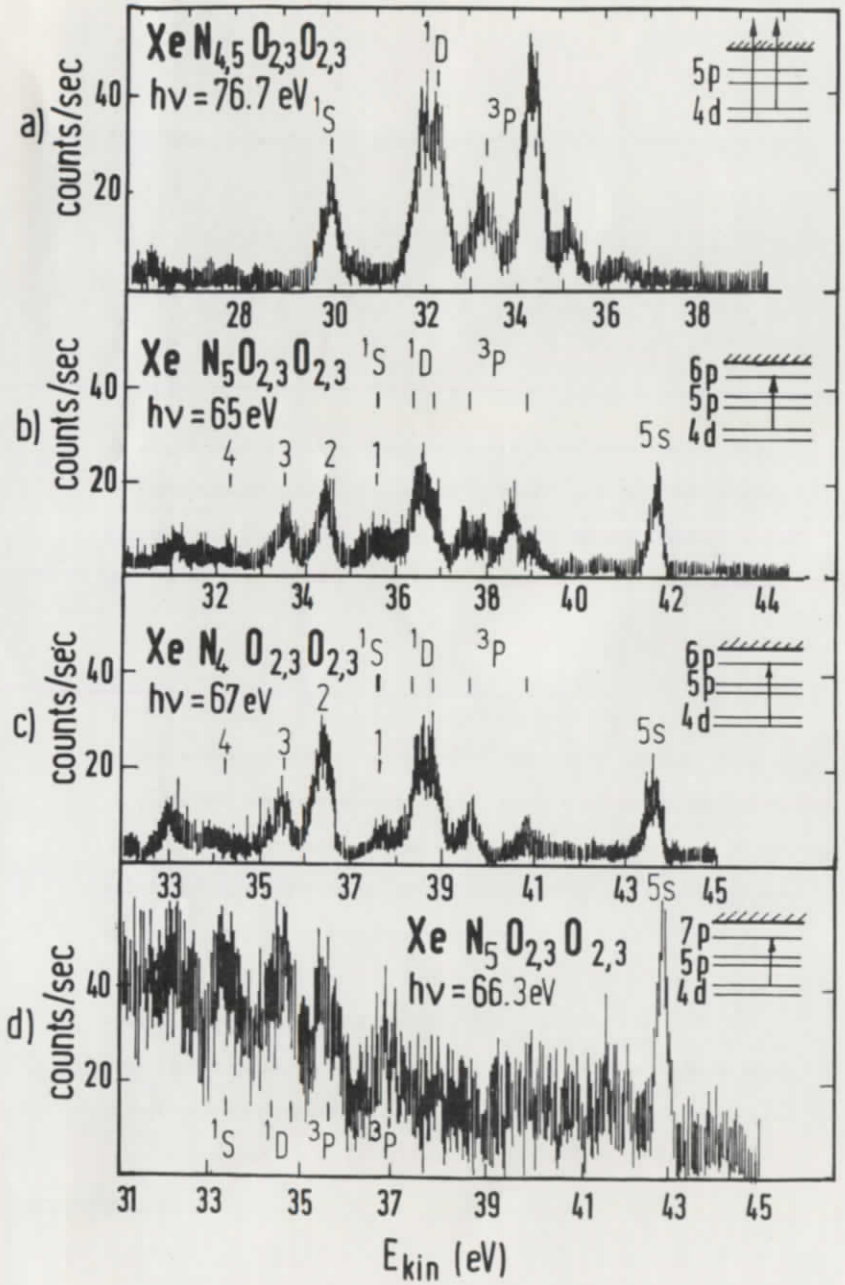
a)
Xe $N_{4,5}O_{2,3}O_{2,3}$
hν = 76.7 eV
$^1S$
$^1D$
$^3P$
5p
4d
counts/sec
b)
Xe $N_5O_{2,3}O_{2,3}$
hν = 65 eV
$^1S$ $^1D$ $^3P$
4 3 2 1
5s
6p
5p
4d
c)
Xe $N_4$ $O_{2,3}O_{2,3}$
hν = 67 eV
$^1S$ $^1D$ $^3P$
4 3 2 1
5s
6p
5p
4d
d)
Xe $N_5O_{2,3}O_{2,3}$
hν = 66.3 eV
5s
7p
5p
4d
$^1S$ $^1D$ $^3P$ $^3P$
$E_{kin}$ (eV)

Fig. 2

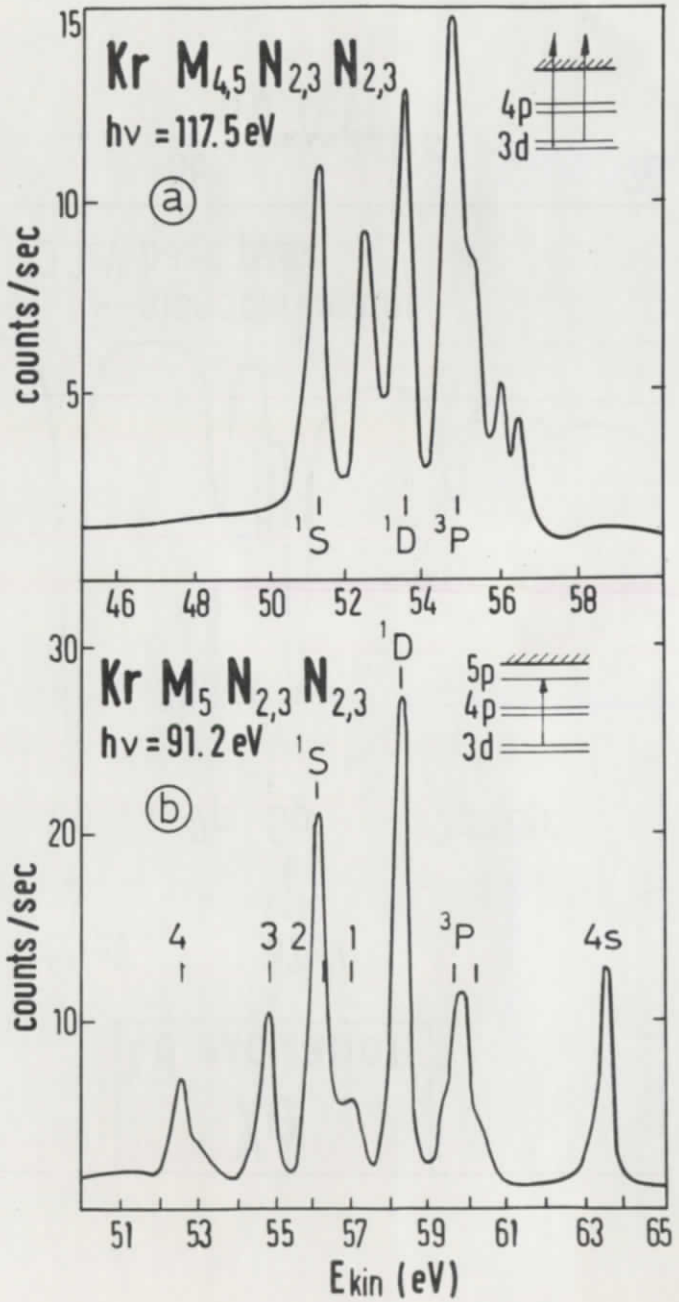
Kr $M_{4,5}N_{2,3}N_{2,3}$
hν = 117.5 eV
a
4p
3d
$^1S$ $^1D$ $^3P$
counts/sec
Kr $M_5N_{2,3}N_{2,3}$
hν = 91.2 eV
b
$^1S$
$^1D$
5p
4p
3d
4 3 2 1
$^3P$
4s
counts/sec
$E_{kin}$ (eV)

Fig. 3