J. Phys. B: At. Mol. Opt. Phys. 36 (2003) 3337-3347

PII: S0953-4075(03)62959-7

Spin polarization transfer in the resonant Auger decay following Kr 3d⁻¹5p photoexcitation

M Drescher¹, T Khalil¹, N Müller¹, S Fritzsche², N M Kabachnik^{3,4} and U Heinzmann¹

¹ Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

² Fachbereich Physik, Universität Kassel, 34132 Kassel, Germany

³ Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

⁴ Institute of Nuclear Physics, Moscow State University, Moscow 119992, Russia

Received 29 April 2003 Published 18 July 2003 Online at stacks.iop.org/JPhysB/36/3337

Abstract

Spin polarization of the resonant Auger electrons is measured following the decay of Kr $3d^{-1}5p$ states resonantly excited by circularly polarized light. A large polarization transfer is found in particular for all strong transitions to the $4s^{-1}4p^{-1}5p$ and $4s^{-2}5p$ states. The experimental results are in excellent agreement with calculations carried out by means of the multiconfiguration Dirac–Fock method.

1. Introduction

The electron spin polarization often carries important information about the dynamics of the photo- and/or Auger electron emission from atoms. Although, in general, the spin polarization of the electrons is more difficult to access than their intensity, it has recently been shown that the electron polarization may reveal rather subtle phenomena like non-dipole contributions in the near-threshold Xe 4p photoionization (Khalil et al 2002). The spin polarization of the Auger electrons has been measured towards a so-called complete experiment for the Auger process where all the Auger amplitudes and their relative phases are to be determined experimentally (Hergenhahn et al 1999, Schmidtke et al 2000, 2001). Experimental progress in electron analysis has been accompanied and stimulated by ever more refined theoretical models for photoionization and Auger decay. A particular challenge is put to the theory by Auger decay following the resonant excitation of core electrons into Rydberg states, because a full description of the possible energy transfer mechanisms between the outgoing Auger electron and the weakly bound outer electrons requires the consideration of many electronic configurations. Therefore, one of the objectives of this work is to study to what extent the theory is capable of predicting and explaining the spin polarization transfer to the Auger electrons following the resonant excitation of a core electron to Rydberg states with circularly polarized photons. To this end, a precision measurement of the spin polarization component P_{trans} parallel to the photon spin was performed for the resonant Kr 3d⁻¹5p Auger decay. In more

detail, we have studied the photoexcitation of the $3d_{5/2}^{-1}5p$ (photon energy $E_{\gamma} = 91.20 \text{ eV}$) and $3d_{3/2}^{-1}5p$ ($E_{\gamma} = 92.42 \text{ eV}$) resonances and their subsequent Auger decay to the final Kr⁺ $4s^{-1}4p^{-1}5p$ and $4s^{-2}5p$ states. These transitions have been investigated in detail both experimentally and theoretically in recent papers (Mursu *et al* 1998, Ueda *et al* 2000, 2003, Kitajima *et al* 2001). The electron spectra have been measured with high resolution and the intensities and angular distributions of Auger electrons have also been determined. Moreover, the alignment of the final ionic states was studied by measuring the angular distributions of the second-step Auger transitions to the Kr²⁺ ions (Ueda *et al* 2000, Kitajima *et al* 2001) as well as the angular correlations between the resonant and the second-step Auger electrons (Ueda *et al* 2003). The *ab initio* calculations, which are carried out within the multiconfiguration Dirac–Fock (MCDF) approach in these recent case studies, describe the experimental data very well.

While a wealth of experimental studies on the resonant excitation of krypton was devoted to the total as well as differential cross sections, no data are yet available for the spin polarization transfer. The measured component of spin polarization P_{trans} is associated with an orientation of the resonant state produced in photoexcitation. Previously a significant dynamical spin polarization, associated with alignment of the resonance, was found for selected lines in the resonant Auger spectra of Xe (Hergenhahn et al 1999) excited by linearly polarized radiation. This is in contrast to the very small dynamical spin polarization of the normal non-resonant Auger electrons. Because of such a difference between the resonant and the non-resonant cases, it will be instructive to test how well the transferred spin polarization of resonant Auger lines can be predicted, starting from the polarization above the ionization threshold and applying simple arguments from the spectator model. In addition, an attempt will be made to combine the experimental data from this work and from the literature to estimate the constraints which are imposed by the experiment to the Coulomb matrix elements describing the Auger decay. Although we have learnt that a complete experiment for the Auger decay process is generally not possible by solely measuring the electron properties (Schmidtke et al 2000, 2001), in some particular cases the experimental angular distribution and spin polarization of emitted electrons limit considerably the range of possible values of the decay amplitudes and their phases.

In the next section we briefly describe the experimental set-up and provide some details of the measurements. Section 3 gives a short account of the underlying theory and our calculations within the MCDF approach. In section 4, we compare the measured spin polarization of the resonant Auger electrons with the calculated values and discuss the implications of these measurements for our understanding of the resonant transitions considered. Finally, the conclusions of this work are summarized in section 5.

2. Experiment

The measurement of the spin polarization transfer for the resonant Auger decay requires a high flux of wavelength-tunable circularly polarized light. Highly circularly polarized radiation, $P_{\text{circ}} > 0.98$, at photon energies around 90 eV was provided by the beamline UE56/2-PGM at BESSY, Berlin. The light intensity was more than doubled by using both sections of the helical undulator simultaneously which, for a 130 meV bandwidth, resulted in a flux of more than 10^{13} photons s⁻¹ in the ionization volume located directly above a gas-inlet tube. The experimental set-up is presented in figure 1. Since the apparatus has already been described previously (Schmidtke *et al* 2001), here we give only a few details pertinent to this particular experiment. Electrons emitted perpendicularly to the light propagation axis ($\theta = 90^{\circ}$) were energy-analysed in a simulated hemispherical electron spectrometer, guided

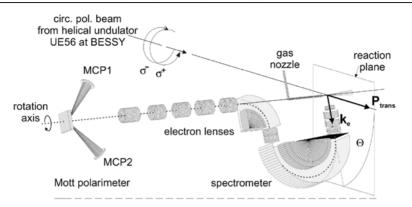


Figure 1. Experimental set-up for measurements of the spin polarization of Auger electrons from krypton gas excited with circularly polarized radiation.

by an electron lens system (Schmidtke *et al* 2000) and subsequently spin-analysed in a spherical retarding-field Mott polarimeter (Müller *et al* 1995) which was operated at 45 keV electron scattering energy. The asymmetry of the backscattering signal in two multichannel-plate detectors located below (N_d) and above (N_u) the electron beam is a measure of the spin polarization transfer:

$$P_{\rm trans} = S_{\rm eff} \frac{N_{\rm d} - N_{\rm u}}{N_{\rm d} + N_{\rm u}},\tag{1}$$

where S_{eff} denotes the analysing power (effective Sherman function) of the polarimeter. By referencing to previous experimental data for the transferred spin polarization of xenon 4d photoelectrons at 94 eV photon energy (Snell *et al* 1999) S_{eff} was determined to be -0.22 ± 0.02 . Magnetic fields were controlled by a combination of Helmholtz coils and μ -metal shields around the spectrometer and the electron lens system. Of utmost importance for minimizing apparatus asymmetries is the opportunity to reverse the helicity of the undulator radiation by shifting the magnet arrays longitudinally. Since the measured asymmetry must exactly reverse its sign correspondingly, apparent asymmetries due to misalignment or residual magnetic fields can efficiently be compensated. In fact, this procedure relies on a fixed beam position upon helicity reversal which was verified for UE56/2. The spin polarization was measured in the line peak with the electron spectrometer resolution set to 350 meV. At backing pressures of about 10⁻⁴ mbar in the vacuum chamber, the count rate in each detector was typically 20 s⁻¹ with an electronic background of typically 5 s⁻¹.

3. Theory

In this section, we explain the method which was used in the calculations of polarization transfer. We consider the resonant Auger process within the conventional two-step approach. In the first step the resonant state of a Kr atom $3d^{-1}5p$ is photoexcited. In the second step, it decays to the final ionic state with emission of an electron. The spin polarization of the emitted electron is determined by the orientation and alignment parameters of the excited atom and by the intrinsic parameters which are characteristic of each of the resonant Auger transitions (Klar 1980, Kabachnik 1981, Kabachnik and Lee 1989, Lohmann 1990, 1998, Balashov *et al* 2000). In the experiment described above, the Auger electrons are detected perpendicular to the direction of the photon beam. In this case the component of the transferred spin polarization

directed along the beam can be presented as

$$P_{\rm trans} = \frac{-\mathcal{A}_{10}\xi_1}{1 - 0.5\mathcal{A}_{20}\alpha_2}.$$
 (2)

Here the orientation \mathcal{A}_{10} and alignment \mathcal{A}_{20} parameters characterize the population of the magnetic sublevels of the primary resonant state (the quantization axis is chosen along the photon beam direction), while the parameters α_2 and ξ_1 are the intrinsic parameters which describe the dynamical properties of the decay process and are related to the reduced matrix elements of the Auger decay. The parameter α_2 describes the angular anisotropy of the Auger emission. The parameter ξ_1 describes, in general, the spin polarization component perpendicular to the electron momentum \mathbf{k}_e in the reaction plane when the reference frame with *z* axis along the direction of electron emission is chosen (Lohmann 1998, Kleiman *et al* 1999, Kabachnik and Sazhina 2002). However, in the geometry of our experiment this component coincides with $-P_{\text{trans}}$. The relationship between intrinsic parameters in the electron and the laboratory frame, respectively, are presented in Schmidtke *et al* (2001). Two further intrinsic parameters which describe the other two spin polarization components are δ_1 (component in the reaction plane) and ξ_2 (component perpendicular to the reaction plane).

The orientation and alignment of the resonant state in the case of photoexcitation by means of circularly polarized light from the J = 0 ground state are well determined and are both model-independent:

$$A_{10} = \pm \sqrt{3/2}$$
 $A_{20} = \sqrt{1/2}$ (3)

(we assume that the photons are completely circularly polarized; the plus sign corresponds to σ^+ circular polarization). On the other hand, in order to calculate the intrinsic parameters one needs the Auger decay amplitudes and therefore the model wavefunctions for the initial and final ionic states.

Simple expressions for the intrinsic parameters in terms of the Auger amplitudes have been obtained recently (Lohmann 1998, Kabachnik and Sazhina 2002). In particular, the parameters α_2 and ξ_1 can be expressed as follows:

$$\alpha_2 = N^{-1} \sum_{jj'} X_{jj'}^2 M_{J_f(l)j} M_{J_f(l')j'}^* \tag{4}$$

$$\xi_1 = N^{-1} \sum_{jj'} C_1(j, j') X^1_{jj'} M_{J_f(l)j} M^*_{J_f(l')j'}$$
(5)

where

$$N = \sum_{j} |M_{J_{f}(l)j}|^{2}$$
(6)

and

$$X_{jj'}^{k} = (-1)^{J_{i}+J_{f}-\frac{1}{2}} \hat{J}_{i}(-1)^{j+j'} \hat{j} \hat{j}'(j\frac{1}{2},j'-\frac{1}{2}|k0) \left\{ \begin{array}{ll} J_{i} & J_{i} & k\\ j & j' & J_{f} \end{array} \right\}.$$
 (7)

The Auger amplitudes $M_{J_f(l)j} \equiv \langle \alpha_f J_f, lj : J_i || V || \alpha_i J_i \rangle$ describe the decay of the initial state $|\alpha_i J_i\rangle$ with the total angular momentum J_i (other quantum numbers characterizing the initial state are denoted as α_i) to the final ionic state $|\alpha_f J_f\rangle$ with the angular momentum J_f and emitted electron with the orbital and the total angular momenta l and j, respectively. In (7), the standard notations for the Clebsch–Gordan and the 6j coefficients are used, and $\hat{j} \equiv \sqrt{2j+1}$. The coefficients $C_1(j, j')$ are given by

$$C_1(j,j') = \frac{1}{4}(-1)^l [(-1)^{j-1/2}(\hat{j})^2 + (-1)^{j'-1/2}(\hat{j}')^2]$$
(8)

where l is even (odd) for even (odd) Auger electron partial waves.

3340

Expressions (4)–(8) are valid for the decay of an isolated resonance with a sharp angular momentum J_i . Therefore, they are directly applicable to the case of the well separated $3d_{5/2}^{-1}5p_{3/2}J_i = 1$ resonance. However, the $3d_{3/2}^{-1}5p$ resonance consists, in fact, of two components with $J_i = 1$ (3d_{3/2}⁻¹5p_{3/2} and 3d_{3/2}⁻¹5p_{1/2} in *jj*-coupling nomenclature). Since the width of the resonances is larger than their separation, they strongly overlap and interfere when excited by a photon. Although one of them is excited 20 times more strongly than the other one (Tulkki et al 1994, Kitajima et al 2001), a proper account of their interference is important for the description of the angular distributions of resonant Auger electrons (Kitajima et al 2001) and their spin polarization. Modification of the formalism, as described above for the case of two overlapping resonances, is straightforward. It can be done, for instance, on the basis of a one-step resonance scattering model by Åberg (1992). A detailed description of this modification for the angular anisotropy parameter α_2 is given by Kitajima *et al* (2001). In exactly the same way, by using the resonance approximation one can generalize the expressions for the spin polarization components for the case of overlapping resonances. The results presented below for the $3d_{3/2}^{-1}$ 5p resonance are calculated in this way, taking into account the interference of the two fine-structure components.

The Auger amplitudes $M_{J_f(l)j}$ have been calculated using the MCDF. A full description of the approximations which are used in the computations is given elsewhere (Kitajima et al 2001). Briefly, both the initial and the final ionic state configuration interactions (FISCI) were taken into account. The initial resonances of a $3d^{-1}5p$ excitation are well described within a (non-relativistic) single-configuration approximation, including the three J = 1levels of interest (Tulkki et al 1994). It is especially important to include FISCI, since the final states for the transitions considered contain three open subshells and therefore are strongly correlated. About 200 configuration state functions (CSF) were used in the calculation; the wavefunction expansion included all CSF of the 4s4p⁵5p configuration as well as the 4s⁰4p⁶5p and $4s^24p^34d5p$ configurations. The admixture of the $4s^24p^34d5p$ configuration is especially important for a good description of the transition energies and the branching ratios. It is also necessary in order to explain the spin-polarization data for a group of transitions at 36.7 eV (see below). The continuum wavefunctions were calculated in the field of the final ion with a proper account of the exchange interaction of the emitted electron with bound-state electrons. The Auger amplitudes were calculated with the help of the RATIP program (Fritzsche 2001) which utilizes the MCDF wavefunctions from the structure code GRASP (Parpia et al 1996). The amplitudes obtained give good agreement with experiment for the energies, intensity ratios and angular anisotropy parameters of the considered resonant Auger transitions (Kitajima et al 2001, Ueda et al 2003). Here, the same amplitudes have been applied for calculations of the polarization parameters by utilizing the RACAH program (Fritzsche 1997, Fritzsche et al 2001).

The results of the calculations of the intrinsic parameters, which describe the angular distribution and spin polarization of some strong transitions, are presented in table 1. Since each peak in the Auger electron spectrum consists of several unresolved lines we present the parameters averaged over the corresponding group. The roman group numbers correspond to the numbering in Kitajima *et al* (2001) and are also shown in figure 2. The numbers of the lines included in each group (column 3) correspond to those used by Mursu *et al* (1998) and Kitajima *et al* (2001). On average 2–4 transitions are included in each group. The α_2 parameter obtained is very close to that calculated earlier (Kitajima *et al* 2001). A few minor differences for some of the groups are due to the fact that, in our experiment, the resolution was lower than in Kitajima *et al* and we included more lines in the averaging. Comparing the results of the calculations for two resonances $3d_{5/2}^{-1}5p$ and $3d_{3/2}^{-1}5p$ we note that the ξ_1 parameters have an

| Group | Final state | Line no. | α2 | ξ1 | δ_1 | ξ2 |
|---------------|---|---------------------------|----------------------------|-------------------------|-------------------------|-----------------------------|
| | | Resonar | nce $3d_{5/2}^{-1}5p$ |) | | |
| II V | $\begin{array}{c} 4s^{-1}4p^{-1}(^{1}P)5p\\ 4p^{-3}4d5p \end{array}$ | 13–15 60–64 | -0.357 -0.361 | -0.678 -0.699 | 0.396 0.393 | -0.0026 0.0263 |
| VI | 4s ⁻² (¹ S)5p ² P | 136–137 | -0.555 | -0.744 | 0.263 | -0.0004 |
| | | Resonar | nce $3d_{3/2}^{-1}5p$ |) | | |
| II V VI | $\begin{array}{l} 4s^{-1}4p^{-1}(^{1}P)5p\\ 4p^{-3}4d5p\\ 4s^{-2}(^{1}S)5p \end{array}$ | 12–15 60–64 135–137 | -0.312 -0.313 -0.457 | 0.591 0.586 0.722 | 0.086 0.086 0.354 | 0.0004 -0.0032 0.0001 |

Table 1. The intrinsic anisotropy and spin-polarization parameters calculated by the MCDF method for some groups of strong lines in the Kr $3d^{-1}$ 5p resonant Auger spectra.

opposite sign, which means a different sign of the polarization transfer for the two spin–orbit components of the hole state. This is similar to the non-resonant photoionization (Cherepkov 1973). It is interesting to note that the predicted value of δ_1 which characterizes the longitudinal polarization for groups II and V of the $3d_{5/2}^{-1}5p$ resonance is five times larger than for the $3d_{3/2}^{-1}5p$ resonance. The ξ_2 parameter, which determines the dynamical spin polarization, is very small for all transitions considered.

4. Results and discussion

Figure 2 presents the experimental spectra and the measured spin-polarization transfer for the resonant Auger electrons from the decay of the $3d_{5/2}^{-1}$ 5p (figure 2(a)) and $3d_{3/2}^{-1}$ 5p (figure 2(b)) resonances. Due to the necessity of maximizing the throughput of the electron spectrometer for achieving reasonable count rates, the energy resolution in our experiment is lower than in the previous measurements by Mursu et al (1998) and Kitajima et al (2001). However, the gross structure of the intensity spectra is very close to those observed in the previous experiments. As expected, the excitation from different fine-structure components results in opposite signs of the electron spin polarization. The absolute value of the polarization is as large as 0.6-0.8. The most striking feature is the small variation of P_{trans} which hardly differs from line to line in spite of their totally different nature. Indeed, lines II and VI are $4s^{-1}4p^{-1}(^{1}P)5p$ and $4s^{-2}(^{1}S)5p$ spectator Auger lines, respectively, while line IV is a $4s^{-1}4p^{-1}(^{1}P)6p$ shake-up satellite of line II, and line V corresponds to a $4p^{-3}4d5p$ configuration satellite. This behaviour of P_{trans} is explained below in the theoretical analysis. In order to maximize the signal, the monochromator resolution was also limited to a 130 meV pass band. For the case of the $3d_{3/2}^{-1}5p \rightarrow 4s^{-1}4p^{-1}(^{1}P)6p$ shake-up satellite this resulted in a noticeable contribution from an excitation of the $3d_{5/2}^{-1}$ 6p transition. This background was taken into account by correcting the spin polarization measured at 92.42 eV photon energy with the spectrally weighted polarization of the $3d_{5/2}^{-1}6p \rightarrow 4s^{-1}4p^{-1}6p$ line ($P_{trans} = 0.46$), as measured at 92.56 eV photon energy. In the same figure we show the results of our MCDF calculations (open squares). The agreement between theory and experiment is very good. We note that the total error indicated in figure 2 is dominated by the uncertainty in determining the analysing power S_{eff} of the Mott polarimeter, while the statistical errors are typically a factor of 5 smaller. Since the former introduces a simultaneous scaling of all data points and will not remove systematical variations, the residual small variations in P_{trans} can be regarded as being significant. The measured and calculated values of the polarization are also listed in table 2.

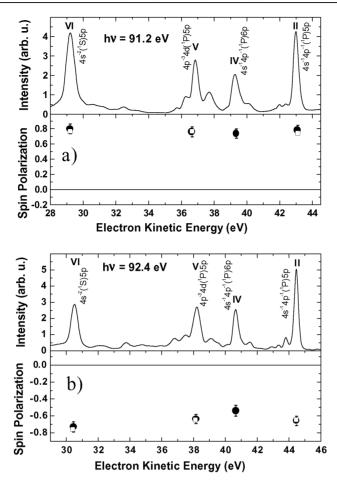


Figure 2. Relative intensity and transferred spin polarization of electrons from the Auger decay of intermediate 5p Rydberg states resonantly excited from the $3d_{5/2}$ (a) and $3d_{3/2}$ (b) fine-structure subshells of krypton atoms. Full circles: experiment; open squares: MCDF calculation.

The last column in the table shows the polarization as calculated in a very simple single partial wave (SPW) model. Consider, for example, line II. The calculations (Mursu *et al* 1998, Kitajima *et al* 2001) show that the main contribution to the intensity of this peak arises from the final state ${}^{2}D_{5/2}$. Moreover, in this transition the partial wave $f_{7/2}$ strongly dominates. If we ignore other possible waves $(f_{5/2}, p_{3/2})$ and consider only one $(f_{7/2})$ then all intrinsic parameters turn out to be independent of matrix elements (see equation (5)) and become pure geometrical quantities, easy to calculate. This fact is well known and has been widely used for the determination of α_{2} parameters (Mehlhorn 1985). It is also valid for the spin polarization parameters (Kabachnik and Lee 1989, Lohmann *et al* 1993). In fact, keeping only one dominant term in the summations ((4)–(6)) one has the intrinsic parameters in the SPW model:

$$\alpha_2 = X_{jj}^2 = (-1)^{J_i + J_f + \frac{1}{2}} \hat{J}_i \hat{j}^2 (j\frac{1}{2}, j - \frac{1}{2}|20) \begin{cases} J_i & J_i & 2\\ j & j & J_f \end{cases}$$
(9)

and

$$\xi_1 = C_1(j,j)X_{jj}^1 = \frac{1}{2}(-1)^{l+j+J_i+J_f}\hat{J}_i\hat{j}^4(j\frac{1}{2},j-\frac{1}{2}|10) \left\{ \begin{array}{ll} J_i & J_i & 1\\ j & j & J_f \end{array} \right\}.$$
(10)

| Group | Final state | Experiment | MCDF | SPW |
|-------|---|----------------------|--------|-------|
| | Resonan | ce $3d_{5/2}^{-1}5p$ | | |
| II | 4s ⁻¹ 4p ⁻¹ (¹ P)5p | 0.780 ± 0.010 | 0.737 | 0.727 |
| IV | $4s^{-1}4p^{-1}(^{1}P)6p$ | 0.733 ± 0.017 | | |
| V | 4p ⁻³ 4d5p | 0.755 ± 0.026 | 0.759 | |
| VI | $4s^{-2}(^{1}S)5p^{2}P$ | 0.795 ± 0.010 | 0.762 | 0.750 |
| | Resonan | ce $3d_{3/2}^{-1}5p$ | | |
| Π | 4s ⁻¹ 4p ⁻¹ (¹ P)5p | -0.660 ± 0.019 | -0.652 | |
| IV | $4s^{-1}4p^{-1}(^{1}P)6p$ | -0.540 ± 0.038 | | |
| V | $4p^{-3}(^{2}D)4d(^{1}P)5p$ | -0.638 ± 0.019 | -0.646 | |
| VI | $4s^{-2}(^{1}S)5p$ | -0.731 ± 0.012 | -0.761 | |

Table 2. The measured and calculated spin polarization component P_{trans} for some groups of strong lines in the Kr 3d⁻¹5p resonant Auger spectra.

Substituting $J_i = 1$, $J_f = 5/2$ and j = 7/2 for the transition considered one gets the values of ξ_1 and α_2 within the SPW model, yielding the transferred polarization $P_{\text{trans}} = -0.727$ which is close to the experiment and the MCDF calculations. One should be cautious, however, with such a comparison, since the MCDF values given in table 2 are averaged over several lines with different J_f , while the SPW value corresponds to a single line only. Nevertheless, we can conclude that one Auger amplitude strongly dominates for the main transition in this line. We note that other partial waves give a very different polarization and even different sign. The dominance of a SPW does not necessarily mean that other partial waves do not contribute at all. The value of the α_2 parameter calculated for this transition by only considering a $f_{7/2}$ wave is -0.505, which is larger than the MCDF and the experimental value of -0.375 (Kitajima et al 2001, Tulkki et al 1994), which clearly indicates the presence of other partial waves. A similar situation occurs also for line VI where the strongest transition in the group is that to the final state ${}^{2}P_{3/2}$ for which the d_{5/2} partial wave dominates. Regarding only this partial wave we easily get $P_{\text{trans}} = 0.750$ which is again close to the experiment and detailed MCDF calculations. The dominance of one partial wave is confirmed by the fact that for almost all considered transitions the dynamical spin polarization parameter ξ_2 is close to zero. It should be exactly zero if only one partial wave contributes (Kabachnik and Sazhina 1984).

The observed similarity of the polarization transfer for the spectator transitions (group II) and shake-modified transitions (group IV) can be qualitatively understood on the basis of a simple sudden-approximation model, where the amplitude of the shake-modified Auger transition differs from the corresponding diagram transition by the overlap factor $\langle 5p|6p \rangle$. This factor cancels out of all intrinsic parameters. Thus, in this rather rough approximation the polarization transfer for groups II and IV should be equal (compare with the discussion for α_2 in Hergenhahn *et al* (1991)). A more refined theoretical treatment is necessary for the explanation of an observed small but distinct difference in polarization satellites (group V) is close to that of the diagram transitions (group II) both in experiment and in theory. These satellites are populated mainly due to the admixture of the diagram line configuration ($4s^{-1}4p^{-1}5p$) and therefore the ratios of the amplitudes and the phases which determine the polarization parameters should be similar for satellites and diagram transitions. Summarizing the above discussion we can state that only small variations of the average polarization transfer for all strong lines in the spectrum are to be expected, which is indeed observed in the experiment.

Recently we have measured the intrinsic spin-polarization parameters for the $M_{4,5}$ – $N_1N_{2,3}$ normal Auger transitions (Schmidtke *et al* 2001). These transitions differ from those which are studied in the present work by the absence of the extra (spectator) electron at the excited 5p state. It is of interest to compare the intrinsic parameters for the resonant Auger and the corresponding normal Auger transitions. As a first approximation we can completely ignore the interaction of the spectator electron with the electrons of the core. This is a so-called gross-spectator model (Kämmerling *et al* 1990). In this model it is possible to obtain a relation (Hergenhahn *et al* 1991) between the anisotropy parameter of a normal Auger transition and the anisotropy parameters of the corresponding resonance Auger transitions summed over the multiplet which appears due to coupling of the vacancy with the spectator electron. This relation can be generalized to any intrinsic parameter. Indeed, using equation (19) from Hergenhahn *et al* (1991) for the matrix elements and a general expression for the intrinsic parameters (Kabachnik and Sazhina 2002) one can easily show that

$$\tau_k^{\Sigma}(\text{res}) = (-1)^{J_i + j_0 + j_1 - k} \hat{J}_i \hat{j}_0 \begin{cases} J_i & J_i & k \\ j_0 & j_0 & j_1 \end{cases} \tau_k(\text{nor})$$
(11)

where τ represent any of the intrinsic parameters, k = 1 for ξ_1 and δ_1 , k = 2 for α_2 and ξ_2 ; j_0 and j_1 are the angular momenta of the vacancy and the spectator electron, respectively, J_i is the angular momentum of the resonant state ($J_i = 1$ in our case) and abbreviations 'res' and 'nor' refer to resonant Auger and normal Auger transitions, respectively. In the particular case of the M5-N1N2.3 Auger decay and the corresponding decay of the resonance $3d_{5/2}^{-1}$ 5p, the relation (11) yields ξ_1^{Σ} (res) = $\sqrt{7/10}\xi_1$ (nor). Experimentally, the ξ_1 parameter for the M₅–N₁N_{2,3} ¹P transition was determined as -0.79 ± 0.10 (Schmidtke *et al* 2001) and -0.84 ± 0.06 (Snell *et al* 2002). Thus for the resonant Auger transitions we get the averaged value of -0.69, in excellent agreement with the value calculated by the MCDF method (see table 1) and in agreement with the present experiment. At first sight this means that the grossspectator model is valid, i.e. the interaction of the spectator electron with the core is indeed negligible. However, it is more likely that this agreement reflects the fact that one partial wave dominates in both the normal and the resonant Auger decay. In fact, if only one partial wave contributes then matrix elements cancel out from the intrinsic parameters at the both sides of equation (11) and it becomes an identity which reflects the sum rule of the angular momentum coupling coefficients. No dynamical information concerning the interactions can then be derived from its fulfilment.

The reported measurement of the spin-polarization transfer complements recent angular correlation measurements for the same transitions (Kitajima et al 2001, Ueda et al 2003). However, the experimental information is still not sufficient for extraction of the Auger decay amplitudes from the experimental data, i.e. for the realization of a complete experiment. Spinpolarization transfer and angular anisotropy yield two experimental parameters. The angular distributions of the cascade Auger electrons measured by Kitajima et al can give, in principle, the third parameter: alignment of the ionic state (final state for the transitions considered). Unfortunately, the strongest second-step transitions which were investigated do not give the alignment in a model-independent way. But even if we had measured it, the three parameters would not have been sufficient for determination of the three (in the general case) complex Auger amplitudes describing the resonance Auger decay. Additional information could be extracted from the coincidence angular correlation measurements in the cascade of Auger transitions (Ueda et al 2003). But again the measured transitions do not permit the extraction of information in a model-independent way. Nevertheless, the measured values limit considerably the possible values of the amplitudes. The dominance of one of the partial waves is an example of such a limitation.

5. Conclusions

The spin-polarization transfer in the emission of resonant Auger electrons after Kr $3d^{-1}5p$ photoexcitation by circularly polarized light has been studied experimentally. We found large spin polarization for all strong lines in the spectra. The polarization is practically independent of the nature of the line. Calculations within the framework of the MCDF approach agree very well with experiment. A qualitative explanation of the results is suggested based on the fact that, for the diagram transitions under investigation, one partial wave dominates. Although a combination of all experimental data concerning the investigated transitions can still not provide a unique determination of the corresponding Auger amplitudes, the measurements limit considerably their possible values. Good agreement of the theoretical values of the spin polarization and anisotropy of the Auger electrons with the experiment indirectly gives information about the amplitudes, confirming that the calculated amplitudes are close to reality.

Acknowledgments

This work was supported by the Deutsche Forschungsgemeinschaft. We acknowledge the support by the BESSY staff. NMK acknowledges the hospitality and financial support of the Fritz-Haber-Institute of the Max-Planck Society.

References

- Åberg T 1992 Phys. Scr. T 41 71
- Balashov V V, Grum-Grzhimailo A N and Kabachnik N M 2000 Polarization and Correlation Phenomena in Atomic Collisions. A Practical Theory Course (New York: Kluwer-Academic) ch 1
- Cherepkov N A 1973 Zh. Eksp. Teor. Fiz. 65 933 (Engl. transl. 1974 Sov. Phys.-JETP 38 463)
- Fritzsche S 1997 Comput. Phys. Commun. 103 51
- Fritzsche S 2001 J. Electron. Spectrosc. Relat. Phenom. 114-116 1155
- Fritzsche S, Inghoff T, Bastug T and Tomaselli M 2001 Comput. Phys. Commun. 139 314
- Hergenhahn U, Kabachnik N M and Lohmann B 1991 J. Phys. B: At. Mol. Opt. Phys. 24 4759
- Hergenhahn U, Snell G, Drescher M, Schmidtke B, Wiedehoft M, Muller N, Becker U and Heinzmann U 1999 Phys. Rev. Lett. 82 5020
- Kabachnik N M 1981 J. Phys. B: At. Mol. Phys. 14 L337
- Kabachnik N M and Lee O V 1989 J. Phys. B: At. Mol. Opt. Phys. 22 2705
- Kabachnik N M and Sazhina I P 1984 J. Phys. B: At. Mol. Phys. 17 1335
- Kabachnik N M and Sazhina I P 2002 J. Phys. B: At. Mol. Opt. Phys. 35 3591
- Kämmerling B, Krässig B and Schmidt V 1990 J. Phys. B: At. Mol. Opt. Phys. 23 4487
- Khalil T, Schmidtke B, Drescher M, Müller N and Heinzmann U 2002 Phys. Rev. Lett. 89 053001
- Kitajima M et al 2001 J. Phys. B: At. Mol. Opt. Phys. 34 3829
- Klar H 1980 J. Phys. B: At. Mol. Phys. 13 4741
- Kleiman U, Lohmann B and Blum K 1999 J. Phys. B: At. Mol. Opt. Phys. 32 309
- Lohmann B 1990 J. Phys. B: At. Mol. Opt. Phys. 23 3147
- Lohmann B 1998 Habilitation Thesis Westfälisher Wilhelms-Universität, Münster
- Lohmann B, Hergenhahn U and Kabachnik N M 1993 J. Phys. B: At. Mol. Opt. Phys. 26 3327
- Mehlhorn W 1985 Atomic Inner-Shell Physics ed B Crasemann (New York: Plenum) p 119
- Müller N et al 1995 J. Electron Spectrosc. Relat. Phenom. 72 187
- Mursu J, Jauhiainen J, Aksela H and Aksela S 1998 J. Phys. B: At. Mol. Opt. Phys. 31 1973
- Parpia F A, Froese Fischer C and Grant I P 1996 Comput. Phys. Commun. 94 249
- Schmidtke B, Khalil T, Drescher M, Müller N, Kabachnik N M and Heinzmann U 2000 J. Phys. B: At. Mol. Opt. Phys. 33 5225
- Schmidtke B, Khalil T, Drescher M, Müller N, Kabachnik N M and Heinzmann U 2001 J. Phys. B: At. Mol. Opt. Phys. 34 4293
- Snell G, Langer B, Drescher M, Muller N, Zimmermann B, Hergenhahn U, Viefhaus J, Becker U and Heinzmann U 1999 Phys. Rev. Lett. 82 2480

Snell G, Langer B, Young A T and Berrah N 2002 *Phys. Rev.* A **66** 022701 Tulkki J, Aksela H and Kabachnik N M 1994 *Phys. Rev.* A **50** 2366

Ueda K, Kabachnik N M, Kitajima M, Okamoto M, Shimizu Y, Chiba H, Hayaishi T and Tanaka H 2000 J. Phys. B: At. Mol. Opt. Phys. 33 L475

Ueda K et al 2003 J. Phys. B: At. Mol. Opt. Phys. 36 319