Relativistic-intermediate-coupling calculations of angular distributions in resonant Auger decay

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The angular-distribution parameters of the resonant Auger transitions induced by photoexcitation have been calculated for the L_{23}-$M_{23}M_{23}$, M_{45}-$N_{23}N_{23}$ and N_{45}-$O_{23}O_{23}$ transitions in Ar, Kr, and Xe, respectively. The calculations are carried out using the multiconfiguration Dirac-Fock method in intermediate coupling with configuration interaction. A two-step model is employed to describe the resonant Auger process. As in the case of normal Auger decay, inclusion of the effect of intermediate coupling removes the major discrepancy between theory based on the spectator model and experiment.

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I. INTRODUCTION

The advances in synchrotron radiation have provided a power tool to study the properties of resonantly excited states. The decays of these autoionizing states are dominated by the resonant Auger transitions which involve inner-shell electrons with the resonantly excited electron remaining in its orbital or being excited into a higher shell [1]. Recently, the Auger decay of the resonantly excited state has been subject to rather intense investigations [1–6]. The experimental work on angular distributions of the resonant Auger electrons in rare gases [7–11] have revealed a large degree of angular anisotropy for many transitions. This unusually large angular anisotropy in $_{18}$Ar was first explained by Cooper [12] using the angular-momentum-transfer theory. Later, Hergenhahn, Kabachnik, and Lohmann [13] treated the resonant Auger transition as a two-step process [14] involving excitation and subsequent Auger decay. They calculated the angular distributions of the resonant Auger transitions for $_{18}$Ar, $_{36}$Kr, and $_{54}$Xe by describing the excited and final states in jK coupling scheme and treating the outer electron as a spectator. Although the results from Hergenhahn, Kabachnik, and Lohmann [13] agree favorably with experiments, large discrepancies exist for a few transitions.

In our previous work [15], we have shown the importance of including the effect of intermediate coupling in the calculations of angular distributions of a normal Auger decay. In this paper, we report on the theoretical calculations of angular anisotropy of the resonant Auger transitions based on a two-step model for Ar, Kr, and Xe with $2p$-$4s$, $3d$-$5p$, and $4d$-$6p$ excitations, respectively. The calculations were carried out using the multiconfiguration Dirac-Fock (MCDF) method [16,17] in intermediate coupling with configuration interaction. The inclusion of intermediate-coupling effect removes the remaining discrepancies between theory and experiment.

II. THEORETICAL METHOD

As in our previous work [15], we treat the resonant Auger decay as a two-step process in which the interference between the resonant and direct ionization channels is ignored. Since the j-j coupling is the natural coupling scheme for the relativistic atomic structure calculation, we employed the j-j coupling scheme in the basis functions and in the derivation of angular-distribution function. The intermediate coupling in the MCDF method can be implemented through the configuration interaction. Under the most common experimental conditions, the angular distribution of Auger electrons induced by a beam of linearly polarized photons can be written in the dipole approximation as [15,18,19]

$$W(\theta)=\frac{W_0}{4\pi}[1+\beta P_2(\cos\theta)] , \tag{1}$$

with the angular-distribution parameter $\beta=\alpha_2 A_{20}$.

Here, W_0 is the total Auger-decay probability per unit time; θ is the angle between the direction of the Auger electrons and the polarization vector which is chosen as the quantization axis and $P_2(\cos\theta)$ is the second Legendre polynomial; A_{20} is the alignment of the excited states along the quantization axis. For exciting to a state with total angular momentum $J=1$ from the ground state with $J=0$ using linearly polarized photons, the value of the alignment parameter A_{20} has been calculated: $A_{20}=-\sqrt{2}$ [13].

The Auger-decay anisotropy parameter α_2 in Eq. (1) is the characteristic of a particular Auger transition, and is given by [15,20]

$$\alpha_L=\sum_{\kappa,\kappa'}(-1)^{J_i+J_f-1/2}(i)^{(l-l')}\cos(\delta_\kappa-\delta_{\kappa'})[l,l',j,j',L,J_i]^{1/2}\begin{Bmatrix} l' & l & L \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} j & j' & L \\ l' & l & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} J_i & J_i & L \\ j' & j & J_f \end{Bmatrix}$$
$$\times\langle J_f jJ_i\|V\|J_i\rangle\langle J_f j'J_i\|V\|J_i\rangle^*\left[\sum_\kappa|\langle J_f jJ_i\|V\|J_i\rangle|^2\right]^{-1} . \tag{2}$$

Here, $\kappa=(l-j)(2j+1)$ is the relativistic quantum number; l and j are the orbital and total angular momentum of the continuum electron; δ_κ is the phase shift; J_i and J_f are the total angular momentum of the initial excited state and the final state reached by Auger decay, respectively; $\langle J_f j J_i \| V \| J_i \rangle$ is the reduced Auger matrix element and $[a,b,c,\ldots]\equiv[(2a+1)(2b+1)(2c+1)\cdots]$. The summation over κ is Eq. (2) includes the summations over l and j.

In most existing experiments, the energy resolution is not good enough to resolve the final fine-structure states. For comparisons with experimental observations of angular-distribution parameter β, the average Auger-decay anisotropy parameter α_2 for a group of unresolved Auger lines is calculated by weighting each α_2 value with its Auger rate,

$$\bar{\alpha}_2=\sum_i W_0(i)\alpha_2(i)\Big/\sum_i W_0(i) \ . \tag{3}$$

The products of these group $\bar{\alpha}_2$ values and A_{20} are used to compare with experiments.

III. NUMERICAL CALCULATIONS

In this work, we performed the relativistic-intermediate-coupling calculations for the resonant Auger transitions for the L_{23}-$M_{23}M_{23}$ of $_{18}$Ar, M_{45}-$N_{23}N_{23}$ of $_{36}$Kr, and N_{45}-$O_{23}O_{23}$ of $_{54}$Xe. The excited states $2p^{-1}4s$, $3d^{-1}5p$, and $4d^{-1}6p$ in Ar, Kr, and Xe, respectively, were created using linearly polarized photons. Here $2p^{-1}$ indicates a hole in the $2p$ subshell. The details for calculating the reduced Auger matrix elements and the Auger anisotropy parameters α_2 using the MCDF model were described in Refs. [15] and [16].

Briefly, the Auger-transition rates and reduced Auger matrix elements were calculated from perturbation theory. The energies and wave functions for bound states were evaluated using the MCDF model with average-level scheme [17]. The inner-shell excited states and the final two-hole states were treated in intermediate coupling with configuration interaction. For example, the basis functions for the final two-hole states in the M_{45}-$N_{23}N_{23}$ resonant Auger transitions of Kr include all states from the $4s^04p^65p$ and $4s^24p^45p$ configurations. There are two $J=1$ states (i.e., $^1P_1$ and $^3P_1$) for the $2p^{-1}4s$ excited states and three $J=1$ states (i.e., $^1P_1$, $^3P_1$, and $^3D_1$) for the $3d^{-1}5p$ and $4d^{-1}6p$ excited states. The

TABLE I. Auger energies (in eV) and Auger rates (in sec^{-1}) for the L_{23}-$M_{23}M_{23}$ resonant Auger transitions in $_{18}$Ar. Numbers in brackets denote powers of 10.

	$2p^{-1}4s(^1P_1)$		$2p^{-1}4s(^3P_1)$	
Final state	Energy	Rate	Energy	Rate
$3p^4(^3P)4s\ ^4P_{5/2}$	213.67	1.40[13]	215.79	2.15[13]
$3p^4(^3P)4s\ ^4P_{3/2}$	213.56	1.48[13]	215.68	1.28[13]
$3p^4(^3P)4s\ ^4P_{1/2}$	213.49	1.49[13]	215.62	2.34[13]
$3p^4(^3P)4s\ ^2P_{3/2}$	213.13	5.68[13]	215.26	2.40[13]
$3p^4(^3P)4s\ ^2P_{1/2}$	213.00	1.84[13]	215.13	2.45[13]
$3p^4(^1D)4s\ ^2D_{5/2}$	211.41	1.43[13]	213.53	7.33[13]
$3p^4(^1D)4s\ ^2D_{3/2}$	211.40	7.46[13]	213.52	2.13[13]
$3p^4(^1S)4s\ ^2S_{1/2}$	209.59	1.93[13]	211.71	2.27[13]

TABLE II. Auger energies (in eV) and Auger rates (in sec^{-1}) for the M_{45}-$N_{23}N_{23}$ resonant Auger transitions in $_{36}$Kr. Numbers in brackets denote powers of 10.

	$3d^{-1}5p(^1P_1)$		$3d^{-1}5p(^3P_1)$		$3d^{-1}5p(^3D_1)$	
Final State	Energy	Rate	Energy	Rate	Energy	Rate
$4p^4(^3P)5p\ ^4P_{5/2}$	61.02	2.30[12]	62.22	2.22[12]	62.25	3.08[11]
$4p^4(^3P)5p\ ^4P_{3/2}$	60.95	4.71[11]	62.16	1.16[12]	62.19	2.00[11]
$4p^4(^3P)5p\ ^4D_{7/2}$	60.79	3.84[11]	62.00	4.46[11]	62.03	7.63[11]
$4p^4(^3P)5p\ ^4P_{1/2}$	60.76	1.12[11]	61.97	2.04[10]	62.00	2.73[9]
$4p^4(^3P)5p\ ^2D_{5/2}$	60.73	1.38[12]	61.94	1.93[11]	61.97	2.14[12]
$4p^4(^3P)5p\ ^2P_{3/2}$	60.46	5.63[12]	61.67	1.71[11]	61.70	1.80[12]
$4p^4(^3P)5p\ ^2P_{1/2}$	60.34	1.55[12]	61.54	1.15[11]	61.57	3.64[9]
$4p^4(^3P)5p\ ^4D_{5/2}$	60.25	2.58[11]	61.46	1.90[12]	61.49	3.00[12]
$4p^4(^3P)5p\ ^4D_{1/2}$	60.24	5.52[11]	61.45	3.50[11]	61.48	3.64[11]
$4p^4(^3P)5p\ ^4D_{3/2}$	60.23	6.00[11]	61.44	3.15[12]	61.47	7.64[11]
$4p^4(^3P)5p\ ^4S_{3/2}$	60.04	1.02[12]	61.25	5.18[11]	61.28	1.38[12]
$4p^4(^3P)5p\ ^2D_{3/2}$	59.99	1.04[12]	61.20	2.02[12]	61.23	1.04[12]
$4p^4(^3P)5p\ ^2S_{1/2}$	59.93	5.70[11]	61.14	3.29[9]	61.17	3.92[11]
$4p^4(^1D)5p\ ^2F_{5/2}$	58.76	6.47[11]	59.97	4.48[12]	60.00	5.92[12]
$4p^4(^1D)5p\ ^2F_{7/2}$	58.71	4.46[12]	59.92	2.04[12]	59.95	3.47[12]
$4p^4(^1D)5p\ ^2P_{3/2}$	58.64	7.95[12]	59.85	4.64[12]	59.88	3.56[12]
$4p^4(^1D)5p\ ^2P_{1/2}$	58.42	2.94[12]	59.63	2.67[12]	59.66	2.04[12]
$4p^4(^1D)5p\ ^2D_{3/2}$	58.39	2.79[12]	59.60	6.14[12]	59.63	3.36[12]
$4p^4(^1D)5p\ ^2D_{5/2}$	58.37	3.92[12]	59.58	5.58[12]	59.61	4.19[12]
$4p^4(^1S)5p\ ^2P_{1/2}$	56.78	1.34[9]	57.99	9.02[12]	58.02	6.38[12]
$4p^4(^1S)5p\ ^2P_{3/2}$	56.75	9.39[12]	57.96	4.43[12]	57.99	1.02[13]

TABLE III. Auger energies (in eV) and rates (in sec^{-1}) for the N_{45}-$O_{23}O_{23}$ resonant Auger transitions in $_{54}$Xe. Numbers in brackets denote powers of 10.

	$4d^{-1}6p(^1P_1)$		$4d^{-1}6p(^3P_1)$		$4d^{-1}6p(^3D_1)$	
Final state	Energy	Rate	Energy	Rate	Energy	Rate
$5p^4(^3P)6p\ ^4P_{5/2}$	39.93	5.01[12]	41.85	4.20[12]	41.90	6.55[11]
$5p^4(^3P)6p\ ^4P_{3/2}$	39.92	6.55[11]	41.84	2.70[12]	41.89	2.00[11]
$5p^4(^3P)6p\ ^4D_{7/2}$	39.71	1.94[12]	41.63	6.49[11]	41.68	2.35[12]
$5p^4(^3P)6p\ ^2D_{5/2}$	39.71	7.00[12]	41.62	9.81[11]	41.68	3.20[12]
$5p^4(^3P)6p\ ^2P_{1/2}$	39.68	1.02[12]	41.60	3.16[10]	41.65	5.25[10]
$5p^4(^3P)6p\ ^2P_{3/2}$	39.34	1.87[13]	41.25	2.00[11]	41.31	3.17[12]
$5p^4(^3P)6p\ ^4P_{1/2}$	38.85	1.05[12]	40.77	1.04[11]	40.82	2.32[11]
$5p^4(^3P)6p\ ^4D_{1/2}$	38.79	1.51[12]	40.70	8.51[10]	40.76	1.68[11]
$5p^4(^3P)6p\ ^4D_{3/2}$	38.73	7.53[12]	40.65	5.49[12]	40.70	8.46[11]
$5p^4(^3P)6p\ ^4D_{5/2}$	38.57	2.72[11]	40.49	3.96[12]	40.54	1.43[13]
$5p^4(^3P)6p\ ^4S_{3/2}$	38.51	4.05[12]	40.42	9.99[12]	40.47	1.92[12]
$5p^4(^3P)6p\ ^2D_{3/2}$	38.40	3.60[12]	40.32	9.97[11]	40.37	2.70[12]
$5p^4(^3P)6p\ ^2S_{1/2}$	38.35	3.54[12]	40.26	3.70[11]	40.32	2.45[11]
$5p^4(^1D)6p\ ^2F_{5/2}$	37.48	6.72[11]	39.39	1.84[13]	39.45	1.11[13]
$5p^4(^1D)6p\ ^2P_{3/2}$	37.42	1.28[13]	39.34	1.64[13]	39.39	1.07[13]
$5p^4(^1D)6p\ ^2F_{7/2}$	37.36	1.24[13]	39.27	3.48[12]	39.33	1.26[13]
$5p^4(^1D)6p\ ^2D_{3/2}$	37.10	7.09[12]	39.01	1.80[13]	39.07	5.91[12]
$5p^4(^1D)6p\ ^2P_{1/2}$	37.08	8.14[12]	38.99	3.37[12]	39.05	7.65[12]
$5p^4(^1D)6p\ ^2D_{5/2}$	37.06	8.00[12]	38.98	1.00[13]	39.03	1.56[13]
$5p^4(^1S)6p\ ^2P_{1/2}$	35.37	3.98[9]	37.29	3.20[13]	37.34	1.02[13]
$5p^4(^1S)6p\ ^2P_{3/2}$	35.29	1.51[13]	37.20	6.62[12]	37.26	3.42[13]

eigenfunctions were obtained by diagonalizing the Hamiltonian matrix which includes the Coulomb and transverse Briet interactions [17].

The reduced Auger matrix elements in Eq. (2) were calculated using the bound-state wave functions corresponding to the initial hole state and the continuum wave functions generated by solving the Dirac-Fock equations in the final two-hole potential. The exchange interaction between the continuum and bound electrons is neglected. The continuum wave function is Schmidt orthogonalized to the bound wave functions. The phase shifts in Eq. (2) were calculated according to a procedure given by Zhang, Sampson, and Clark [21].

IV. RESULTS AND DISCUSSIONS

We have calculated the resonant Auger transition rates and angular distribution-parameter α_2 for the excited states $2p^{-1}4s$ in Ar, $3d^{-1}5p$ in Kr, and $4d^{-1}6p$ in Xe using the MCDF method in intermediate coupling with configuration interaction. The results for the Auger energies and rates are listed in Tables I–III. The initial and final states are identified by their dominant components in LS coupling obtained by performing coupling transformation from our j-j into LS basis set [17]. For Ar, the $2p_{3/2}^{-1}4s\ J=1$ and $2p_{1/2}^{-1}4s\ J=1$ states can be identified as $2p^{-1}4s\ ^1P_1$ and $^3P_1$, respectively. The $3d_{5/2}^{-1}5p_{3/2}\ J=1$, $3d_{3/2}^{-1}5p_{1/2}\ J=1$, and $3d_{3/2}^{-1}5p_{3/2}\ J=1$ states of Kr can be associated with $3d^{-1}5p\ ^1P_1$, $^3P_1$, and $^3D_1$, respectively. The same is true for the $4d^{-1}6p$ excited states of Xe. The energy splittings among the final states agree quite well with optical data [22] while the absolute Auger energies differ from the experimental values [7] by amounts less than 1 eV. These discrepancies are mainly due to the residual errors in the treatment of electron correlation. The relative line intensities for the $^1P_1$ initial state from the present work agree well with the angle-integrated experimental intensities [7] for Ar and Kr. For $4d^{-1}6p\ ^1P_1$ excited state in Xe, the theory deviates from experiment by 50% in lines 1c and 3a [7].

TABLE IV. The Auger anisotropy parameter α_2 for the L_{23}-$M_{23}M_{23}$ resonant Auger transitions in $_{18}$ Ar.

Final state	$2p^{-1}4s(^1P_1)$	$2p^{-1}4s(^3P_1)$
$3p^4(^3P)4s\ ^4P_{5/2}$	−0.177	−0.136
$3p^4(^3P)4s\ ^4P_{3/2}$	0.619	0.573
$3p^4(^3P)4s\ ^4P_{1/2}$	−1.166	−1.273
$3p^4(^3P)4s\ ^2P_{3/2}$	0.691	0.558
$3p^4(^3P)4s\ ^2P_{1/2}$	0.616	0.510
$3p^4(^1D)4s\ ^2D_{5/2}$	−0.902	−0.183
$3p^4(^1D)4s\ ^2D_{3/2}$	−0.212	0.610
$3p^4(^1S)4s\ ^2S_{1/2}$	−0.695	−0.009 81

The angular anisotropy parameters α_2 for the L_{23}-$M_{23}M_{23}$, M_{45}-$N_{23}N_{23}$, and N_{45}-$O_{23}O_{23}$ resonant Auger transitions in Ar, Kr, and Xe, respectively, are given in Tables IV–VI. The α_2 parameters vary widely among different final states with values ranging from +0.707 to −1.273 which yields large β values from −1 to +1.8.

In Tables VII–IX, we compare the experimental measured angular-distribution parameters [7–11] with the theoretical predictions from Hergenhahn, Kabachnik, and Lohmann [13] and the present work. The line num-

TABLE V. The angular anisotropy parameter α_2 for the M_{45}-$N_{23}N_{23}$ resonant Auger transitions in $_{36}$Kr.

Final state	$3d^{-1}5p(^1P_1)$	$3d^{-1}5p(^3P_1)$	$3d^{-1}5p(^3D_1)$
$4p^4(^3P)5p\ ^4P_{5/2}$	0.707	0.706	0.620
$4p^4(^3P)5p\ ^4P_{3/2}$	−0.709	−0.593	−0.558
$4p^4(^3P)5p\ ^4D_{7/2}$	0.571	−0.228	−0.224
$4p^4(^3P)5p\ ^4P_{1/2}$	−0.300	−0.890	0.162
$4p^4(^3P)5p\ ^2D_{5/2}$	0.707	0.264	0.705
$4p^4(^3P)5p\ ^2P_{3/2}$	−0.581	0.270	−0.479
$4p^4(^3P)5p\ ^2P_{1/2}$	−0.601	−0.588	0.208
$4p^4(^3P)5p\ ^4D_{5/2}$	0.543	0.662	0.656
$4p^4(^3P)5p\ ^4D_{1/2}$	−0.731	−0.716	−0.699
$4p^4(^3P)5p\ ^4D_{3/2}$	0.636	−0.504	0.113
$4p^4(^3P)5p\ ^4S_{3/2}$	0.270	−0.125	−0.532
$4p^4(^3P)5p\ ^2D_{3/2}$	−0.671	0.307	−0.512
$4p^4(^3P)5p\ ^2S_{1/2}$	−0.630	−0.391	−0.671
$4p^4(^1D)5p\ ^2F_{5/2}$	0.606	0.0347	0.668
$4p^4(^1D)5p\ ^2F_{7/2}$	0.0347	0.490	0.486
$4p^4(^1D)5p\ ^2P_{3/2}$	−0.210	0.0486	−0.643
$4p^4(^1D)5p\ ^2P_{1/2}$	−0.876	−0.642	−0.607
$4p^4(^1D)5p\ ^2D_{3/2}$	0.205	−0.535	0.418
$4p^4(^1D)5p\ ^2D_{5/2}$	0.609	0.394	−0.807
$4p^4(^1S)5p\ ^2P_{1/2}$	−0.690	−0.710	−0.702
$4p^4(^1S)5p\ ^2P_{3/2}$	−0.593	0.561	0.496

TABLE VI. The angular anisotropy parameter α_2 for the N_{45}-$O_{23}O_{23}$ resonant Auger transitions in $_{54}$Xe.

Final state	$4d^{-1}6p(^1P_1)$	$4d^{-1}6p(^3P_1)$	$4d^{-1}6p(^3D_1)$
$5p^4(^3P)6p\ ^4P_{5/2}$	0.707	0.683	0.164
$5p^4(^3P)6p\ ^4P_{3/2}$	−0.696	−0.317	−0.278
$5p^4(^3P)6p\ ^4D_{7/2}$	0.688	−0.103	−0.0992
$5p^4(^3P)6p\ ^2D_{5/2}$	0.707	−0.0136	0.673
$5p^4(^3P)6p\ ^2P_{1/2}$	−0.152	0.0247	0.301
$5p^4(^3P)6p\ ^2P_{3/2}$	−0.720	0.669	−0.721
$5p^4(^3P)6p\ ^4P_{1/2}$	−0.680	−0.697	−0.712
$5p^4(^3P)6p\ ^4D_{1/2}$	−0.547	−0.604	−0.473
$5p^4(^3P)6p\ ^4D_{3/2}$	−0.462	−0.538	−0.0380
$5p^4(^3P)6p\ ^4D_{5/2}$	0.234	0.675	0.677
$5p^4(^3P)6p\ ^4S_{3/2}$	−0.675	−0.211	−0.646
$5p^4(^3P)6p\ ^2D_{3/2}$	0.608	−0.728	−0.513
$5p^4(^3P)6p\ ^2S_{1/2}$	−0.661	−0.661	−0.635
$5p^4(^1D)6p\ ^2F_{5/2}$	0.608	0.308	0.703
$5p^4(^1D)6p\ ^2P_{3/2}$	−0.0517	−0.194	−0.508
$5p^4(^1D)6p\ ^2F_{7/2}$	−0.0366	0.467	0.466
$5p^4(^1D)6p\ ^2D_{3/2}$	0.374	−0.585	0.641
$5p^4(^1D)6p\ ^2P_{1/2}$	−0.924	−0.602	−0.573
$5p^4(^1D)6p\ ^2D_{5/2}$	0.624	0.485	−0.561
$5p^4(^1S)6p\ ^2P_{1/2}$	0.0984	−0.709	−0.700
$5p^4(^1S)6p\ ^2P_{3/2}$	−0.599	0.616	0.500

TABLE VII. Angular-distribution parameter β of resonant Auger decay for $2p_{3/2}$−$4s\ ^1P_1$ excitation of $_{18}$Ar.

		Theory		Expt.		
Peak	Final state	Present work	Hergenhahn *et al.*[b]	I[c]	II[d]	III[e]
1	$3p^4(^3P)4s$	−0.474	−0.496	−0.53		−0.46(10)
2	$3p^4(^1D)4s$	0.456	0.417	0.36,0.48	0.6	0.55(10)
3	$3p^4(^1S)4s$	0.983	1.0	0.39,0.66	1.0[a]	1.09(10)
1a	$3p^4(^3P)4s\ ^4P$	0.344	0.525	0.23	0.3	
1b	$3p^4(^3P)4s\ ^2P$	−0.951	−0.941	−0.69	−0.9	

[a]By assumption.
[b]From Ref. [13].
[c]From Ref. [7] (two sets of data).
[d]From Ref. [8].
[e]From Ref. [10].

TABLE VIII. Angular-distribution parameter β of resonant Auger decay for $3d_{5/2}$−$5p_{3/2}\ ^1P_1$ excitation of $_{36}$Kr.

		Theory		Expt.		
Peak	Final state	Present work	Hergenhahn *et al.*[b]	I[c]		II[d]
1a	$4p^4(^3P)5p\ ^4P_{5/2},^4P_{3/2}$	−0.66	0.007	−0.89	−0.73	−0.76(2)
1b	$4p^4(^3P)5p\ ^4D_{7/2},^4P_{1/2},^2D_{5/2}$	−0.88	−0.15	−0.98	−0.11	−0.87(2)
1c	$4p^4(^3P)5p\ ^2P_{3/2},^2P_{1/2}$	0.83	0.94	0.62	0.35	0.77(6)
1d	$4p^4(^3P)5p\ ^4D_{5/2},^4D_{3/2},^4D_{1/2}$	−0.12	0.883	0.24	0.59	0.04(5)
1e	$4p^4(^3P)5p\ ^4S_{3/2},^2D_{3/2},^2S_{1/2}$	0.42	0.100	0.19	0.31	0.31(6)
2a	$4p^4(^1D)5p\ ^2F_{5/2},^2F_{7/2},^2P_{3/2}$	0.12	−0.144	−0.06	0.00	0.27(3)
2b	$4p^4(^1D)5p\ ^2P_{1/2},^2D_{3/2},^2D_{5/2}$	−0.056	−0.369	−0.12	0.1	0.05(3)
4	$4p^4(^1S)5p\ ^2P_{3/2}$	0.84	0.80	0.73[a]	0.46	

[a]Value from a different data set.
[b]From Ref. [13].
[c]From Ref. [7] (two sets of data).
[d]From Ref. [11].

TABLE IX. Angular-distribution parameter β of resonant Auger decay for $4d_{5/2}-6p_{3/2}\ ^1P_1$ excitation of $_{54}$Xe.

Peak	Final state	Theory: Present work	Theory: Hergenhahn *et al.*[b]	Expt.: I[c]	Expt.: II[d]	Expt.: III[c]
1a	$5p^4(^3P)6p\ ^4P_{5/2},^4P_{3/2}$	−0.770	0.002	−0.88	−0.67(5)	−0.60(3)
1b	$5p^4(^3P)6p\ ^4D_{7/2},^2D_{5/2},^2P_{1/2}$	−0.870	−0.478	−0.93	−0.93(3)	−0.90(2)
1c	$5p^4(^3P)6p\ ^2P_{3/2}$	1.018	1.014	0.82	1.35(6)	1.31(2)
2a	$5p^4(^3P)6p\ ^4P_{1/2},^4D_{1/2},^4D_{3/2}$	0.703	0.859	0.26	0.89(6)	0.58(2)
2b	$5p^4(^3P)6p\ ^4D_{5/2},^4S_{3/2},^2D_{3/2},^2S_{1/2}$	0.348	0.100	0.16	0.45(6)	0.54(3)
3a	$5p^4(^1D)6p\ ^2F_{5/2},^2P_{3/2},^2F_{7/2}$	0.0386	−0.132	−0.02	0.55(5)	0.23(2)
3b	$5p^4(^1D)6p\ ^2D_{3/2},^2P_{1/2},^2D_{5/2}$	−0.0074	−0.081	−0.09	0.46(5)	0.33(5)
5	$5p^4(^1S)6p\ ^2P_{3/2}$	0.847	0.8	0.51	1.26(14)	0.83(5)
6	$5p^4(^1D)7p$	0.0168[a]	−0.10[a]	−0.03		0.12(6)
9	$5p^4(^1S)7p$	0.847[a]	0.8[a]			0.76(3)

[a]Calculated using the values for $6p$ excitation.
[b]From Ref. [13].
[c]From Ref. [7].
[d]From Ref. [10].
[e]From Ref. [9].

bers in these tables are denoted according to Ref. [7]. Hergenhahn, Kabachnick, and Lohmann carried out the theoretical calculations of angular distributions of resonant Auger transitions using the spectator model in the jK coupling scheme. In this coupling scheme, the total angular momentum of the final two holes couples with the orbital angular momentum of the excited electron to yield an intermediate angular momentum K which then couples with the spin of the excited electron to give a total angular momentum of the state. In this approximation, the excited electron enters the calculations through the coupling coefficient and the effect of intermediate coupling among the jK coupled states is neglected.

For $2p_{3/2}$-$4s$ excitation in Ar, our results improve the agreement between theory and experiment. In the case of $3d_{5/2}\rightarrow 5p$ in Kr, our intermediate-coupling results differ considerably from the spectator model [13] except lines 1c and 4. For line 1a, the spectator model yields a near-zero value in strong disagreement with the large negative observed value. On the other hand, our calculation including the effect of intermediate coupling gives a large negative β parameter which agrees very well with the experiments. For peak 1d which is a blend of $4p^4(^3P)5p\ ^4D_{5/2,3/2,1/2}$ states our MCDF model predicts a small negative value (-0.12) while the calculations of Hergenhahn, Kabachnik, and Lohmann yield a large positive number (0.883). On the experimental side, Caldwell [11] gave a value of 0.04 while Carlson *et al.* [7] obtained two β values of 0.24 and 0.59. A closer look at the final-state energy levels reveals that the $4p^4(^3P)5p\ ^2P_{1/2}$ state lies 0.09 eV on the blue side of $^2P_{3/2}$ state and 0.12 eV on the red side of $^4D_{5/2}$ state [22]. A 20% contribution from the $^2P_{1/2}$ state to the peak 1d would give a small positive β value. Overall, our theoretical results achieve very good agreement with recent experiments from Caldwell [11].

For the $4d_{5/2}$-$6p$ excitation in Xe, the present MCDF calculations in intermediate coupling remove the discrepancy between the existing theory [13] and experiments [7,9,10] for peak 1a. In addition, the present work also improves the agreement between theory and experiment for lines 1b and 2b. Since different experiments give quite different results for lines 3a and 3b, it is rather difficult to assess the performance of the theory. In general, our theoretical values agree very well with the experimental findings from Becker *et al.* [10] and Kämmerling, Krässig, and Schmidt [9] except line 3b which agrees better with experimental results from Carlson *et al.* [7]. The excitation of $3d_{3/2}$ to $5p$ or $4d_{3/2}$ to $6p$ gives rise to two $J=1$ states (i.e., $^3P_1$ and $^3D_1$). Since we do not know whether these two states were excited coherently or incoherently, we will not attempt to carry out further analysis for the $3d_{3/2}$-$5p$ and $4d_{3/2}$-$6p$ excitations.

In summary, we have carried out relativistic-intermediate-coupling calculations of angular-distribution parameters in resonant Auger transitions induced by photoexcitation for Ar, Kr, and Xe. We found that inclusion of the effect of intermediate coupling in our MCDF calculations removes the major discrepancy between the predictions from the spectator model and experiment.

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