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Resonances of the photoelectron spin-polarization parameters in the 5*p* autoionization range of xenon

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The spin-polarization parameters for photoelectrons from xenon atoms have been measured in the wavelength range between 96 and 100 nm in an angle-resolving experiment using circularly polarized synchrotron radiation. Theoretical calculations (relativistic random-phase approximation and multichannel quantum defect theory) generally reproduce the wavelength dependence of the parameters, but there are some systematic deviations from the experimental data.

The photoionization of free xenon atoms in the vacuum-ultraviolet (vuv) range has been the subject of extensive experimental work with tunable light sources as well as with resonance line radiation.[1] In contrast with the open continuum region above the second ionization threshold of the 5*p* shell at 92.2 nm, where a large number of measurements of the photoionization cross section,[2] the asymmetry parameter β,[3] and also data for the spin-polarization parameters of photoelectrons[4-6] have been reported, experimental activity in the autoionization range between the $^2P_{3/2}$ and $^2P_{1/2}$ ionization thresholds concentrated mainly on cross-section measurements.[7-10] There also exist data for the spin polarization A (parallel to the photon spin) of the angle-integrated photoelectron flux obtained with circularly polarized synchrotron radiation.[4,5] The only angle-resolved measurements in this region have been carried out by Samson and Gardner,[11] who investigated the variation of the asymmetry parameter β of the differential cross section in the wavelength range from 95.6 to 101.5 nm. Recently, Morioka *et al.*[12] determined β values from an electron spectrum recorded with a steradiancy analyzer, taking into account the dependence of the transmission function of the analyzer upon β.

Theoretical treatments of the photoionization in the autoionization range of xenon are based on the multichannel quantum defect theory (MQDT), usually employing empirically determined MQDT parameters.[13-16] An *ab initio* calculation of these parameters has been performed by Johnson and co-workers[17] in relativistic random-phase approximation (RRPA). Measurements of the photoelectron spin polarization are assumed to provide sensitive tests of the MQDT parameters.[17]

It is the purpose of this Rapid Communication to present the results of the first spin-, angle-, and energy-resolved measurements of the photoelectron emission using circularly polarized radiation in the autoionization range of xenon, and to compare these data with the theoretical predictions.

We have measured the electron spin-polarization components[6] $A(\theta)$ parallel to the photon momentum and $P_\perp(\theta)$ normal to the reaction plane (spanned by photon and electron momentum) for several different photoelectron emission angles θ, where θ is the angle between the momenta of the incoming photon and the outgoing photoelectron. The angular dependence of $A(\theta)$ for completely circularly polarized radiation is given by[6]

$$A(\theta)=\gamma\frac{A-\alpha P_2(\cos\theta)}{1-\frac{1}{2}\beta P_2(\cos\theta)}\ , \tag{1}$$

where $\gamma=+1$ for right-handed (σ^+) and $\gamma=-1$ for left-handed (σ^-) circular polarization. $P_2(\cos\theta)=\frac{3}{2}\cos^2\theta-\frac{1}{2}$ is the second Legendre polynomial. $A(\theta)$ is characterized by the asymmetry parameter β of the differential cross section and by the spin parameters A and α, where A is the angle-integrated spin-polarization transfer. The parameter A can be measured in an angle-integrating experiment as the spin polarization of the total photoelectron flux,[4,5] or in an angle-resolving experiment as the spin polarization $A(\theta_m)$ at the so-called "magic angle" $\theta_m=54.7°$, where the second Legendre polynomial vanishes. The parameter α may be interpreted as the asymmetry parameter of the spin-polarization transfer.[6] In practice, A and α have been determined from the values of $A(\theta)$ for several different angles θ as the result of a least-squares fit on the basis of Eq. (1).

The angular dependence of $P_\perp(\theta)$ does not depend upon the helicity of the ionizing radiation and is given by the following equation, which also holds when unpolarized light is used:[13,18]

$$P_\perp(\theta)=\frac{2\xi\sin\theta\cos\theta}{1-\frac{1}{2}\beta P_2(\cos\theta)}\ . \tag{2}$$

This spin-polarization component is characterized by the spin parameter ξ, which (in analogy to former measurements in the open continuum with unpolarized radiation[18]) has been determined from the spin polarization $P_\perp(\theta_m)=2\xi\sin\theta_m\cos\theta_m$ measured at the magic angle.

The measurements have been performed using circularly polarized synchrotron radiation from the electron storage ring at the Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (BESSY) in combination with a rotatable electron-spectrometer system and a high-energy Mott spin detector. The apparatus has been described earlier in some detail[6] and we only briefly describe the main features.

The synchrotron radiation is dispersed by a 6.5-m normal-incidence monochromator (Monk-Gillieson type),[19] with the electron beam in the storage ring being the virtual entrance slit, resulting in a bandpass of 0.5 nm in first order with a 1200-l/mm grating. Radiation emitted above or below the storage-ring plane, which has positive or negative helicity, respectively, can be selected by apertures movable in vertical direction. In order to resolve the structure in the autoionization range, second-order radiation ($\Delta\lambda = 0.25$ nm) had to be used. This was possible due to the excellent running conditions of the storage ring BESSY, now routinely achieving stored beam currents of 600 mA, which results in an enhancement of the light intensity by a factor of 3 compared with former experiments.[6] The photon flux of second-order radiation at 100 nm of circularly polarized light available behind the exit slit was of the order of 10^{11} photons/s. The intensity loss of about 10^{-3} associated with spin-polarization analysis resulted in count rates between 3 and 20 s^{-1} in the Mott detector, one order of magnitude more than the corresponding background.

As electron-scattering cross sections for xenon atoms amount to between 100 and 1000 Mb for kinetic energies below 1 eV,[20] high target pressure may lead to systematic errors in angle-resolving experiments. We have therefore measured the photoelectron intensity and the photoelectron spin-polarization $A(90°)$ as function of the background pressure in the vacuum chamber for photoelectrons of 300 meV kinetic energy, the background pressure being a mea-

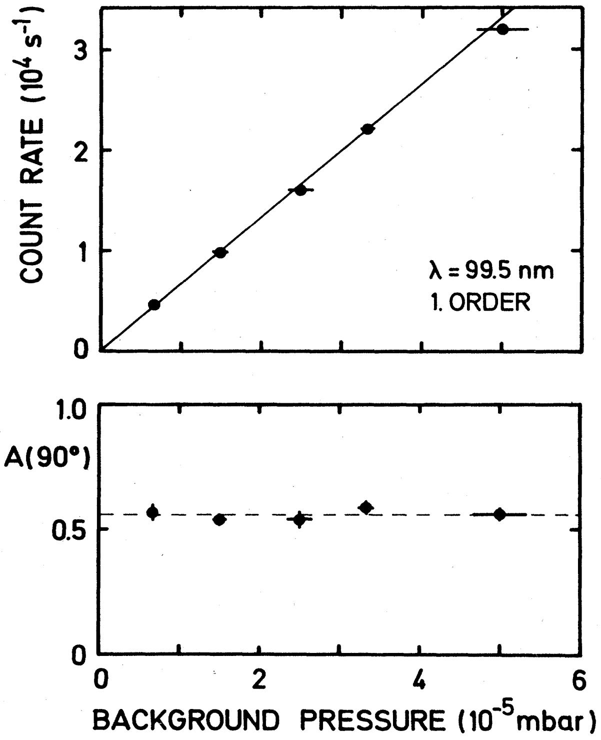

FIG. 1. Photoelectron intensity (upper part) and spin polarization $A(90°)$ (lower part) as functions of the background pressure, which is a measure of the target density, for photoelectrons from the $5p$ shell of xenon at a wavelength of 99.5 nm. The full and dashed lines are drawn to guide the eye.

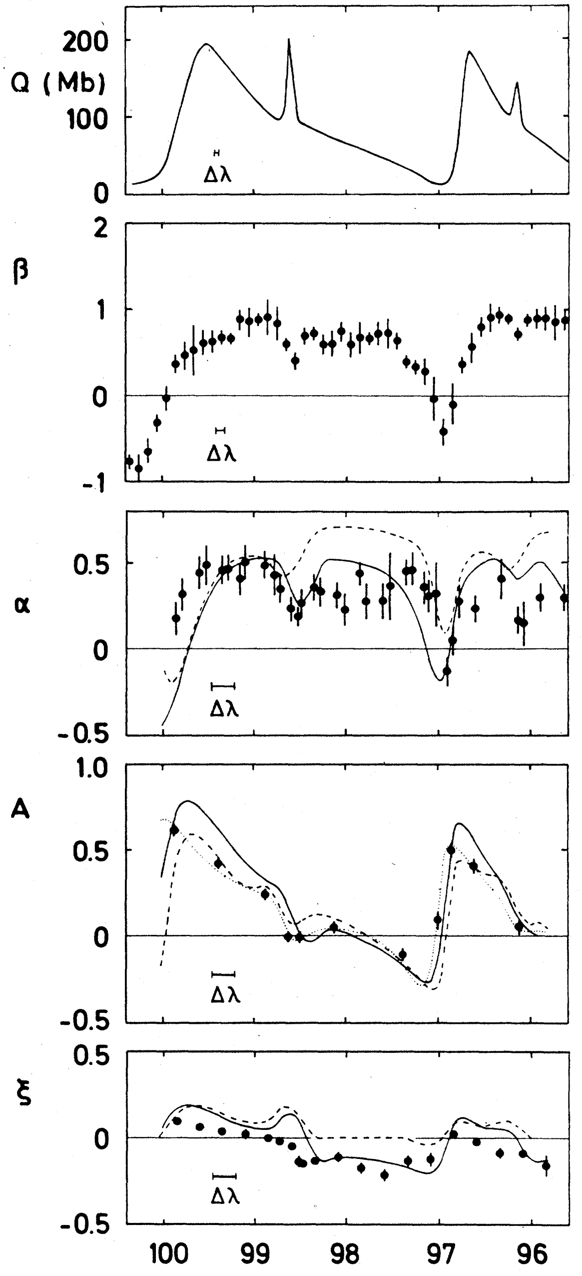

FIG. 2. Cross section Q (Ref. 7) asymmetry parameter β (Ref. 11) and spin parameters α, A, and ξ for the $5p$ autoionization of xenon. The full and dashed curves for the spin parameters represent RRPA (Ref. 17) and semiempirical MQDT (Ref. 13) calculations, respectively, convoluted with the experimental bandwidth of $\Delta\lambda = 0.25$ nm. The dotted curve for A is based on experimental spin-polarization data of the angle-integrated photoelectron flux, convoluted to correspond to the resolution used in this work.

sure of the target intensity. The results are given in Fig. 1 and show no pressure dependence of the spin polarization, whereas the linear increase of the count rate with background pressure indicates the linear increase of the target density. The measurements reported in this Rapid Communication have been performed at background pressures less than 3×10^{-5} mbar.

The experimental results for α, A, and ξ obtained from spin-polarization measurements in the wavelength range between 96 and 100 nm are shown in Fig. 2, together with the photoionization cross section Q measured by Huffman, Tanaka, and Larrabee[7] ($\Delta\lambda = 0.05$ nm), and the asymmetry parameter β measured by Samson and Gardner[11] ($\Delta\lambda = 0.1$ nm). The wavelength calibration of the monochromator was checked at the narrow s resonance in the cross section at 98.6 nm (Ref. 9) to be accurate within ±0.05 nm. The dotted curve for the spin parameter A, based on experimental spin-polarization data of the angle-integrated photoelectron flux[4,5] with a resolution of $\Delta\lambda = 0.05$ nm, is the result of a convolution of these data corresponding to the resolution used in this work. The agreement between the values for A determined from the angle-integrating and from the angle-resolving experiment is good. All spin parameters show pronounced resonance structures. Although the sharp s resonance at 98.6 nm could not be completely resolved using the bandwidth of 0.25 nm, it clearly shows up as a minimum in α and A.

Comparison with theoretical results only makes sense when the limited experimental resolution is taken into account. Therefore, the values for the spin parameters resulting from the semiempirical MQDT calculation by Lee[13] and from the *ab initio* RRPA calculation by Johnson, Cheng, Huang, and LeDourneuf[17] have been convoluted with the experimental bandwidth of 0.25 nm. They are given in Fig. 2 as dashed and full curves, respectively.

The overall agreement in the structure and in the absolute values of the spin parameters between theory and experiment is generally very good. We note, however, that although the position of the sharp s resonance in the cross section and the corresponding features in the other photoionization parameters are very well reproduced by the calculations, the experimental values for the broad d resonance at about 99.5 nm are systematically shifted towards longer wavelengths by approximately 0.3 nm. This discrepancy between theory and experiment concerning the relative position of s and d resonances, which also appears in the spectral behavior of β (Ref. 11) and A (Refs. 4 and 5), is confirmed by the angle-resolved spin-polarization measurements. Johnson *et al.*[17] see the reason for this discrepancy in the limited correlation included in their RRPA calculation. In particular, they compare two calculations, one including correlations from the $5p$ shell only, the other, which results in closer agreement with the experimental data, taking into account the intershell correlations from the $5p$, $5s$, and $4d$ shells. The inability of the semiempirical MQDT calculation[13] to reproduce correctly the relative position of s and d resonances has been attributed[11] to the fact that the theoretical MQDT parameters are extracted from photoabsorption and cross-section measurements, i.e., by fitting resonance profiles, which is a difficult task especially for the broad d resonances, where maximum and minimum are not sharp spectral features. Further discrepancies between theoretical and experimental data appear for the spin parameter ξ. This may be due to the fact that the theoretical expression for ξ contains the sine of the phase-shift differences describing the continuum channels, whereas in the expressions for the other spin parameters and the β parameter, only the cosine of the phase differences appears. Small phase differences may therefore strongly affect the spin parameter ξ, whereas the other spin parameters are less sensitive to these quantities.

Generally, the experimental data for the spin parameters ξ and α are better reproduced by the RRPA calculation than by the semiempirical MQDT results; for the spin parameter A the comparison slightly favors the semiempirical calculation. This may be caused by the fact that the MQDT calculation is based on experimental cross-section data which contain no information on the phase-shift differences. ξ and α, however, contain all phase-shift differences between the three transition matrix elements for the $d_{5/2}$, $d_{3/2}$, and $s_{1/2}$ continua, whereas A contains only the $d_{5/2}$-$d_{3/2}$ phase difference and mainly is given by the amplitudes of the transition matrix elements.

Finally, it is worth noting that the measured spin parameters together with the existing photoionization cross-section data form a "complete" set of observables to characterize the photoionization in the wavelength range covered; the experimental quantities shown in Fig. 2 allow the determination of "experimental" transition matrix elements and phase-shift differences for the photoionization of xenon atoms in the autoionization range. This determination is in progress and is to be discussed in a forthcoming publication.

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[1] For a review, see, e.g., J. A. R. Samson, in *Handbuch der Physik*, edited by W. Mehlhorn (Springer, Berlin, 1982), Vol. 31, p. 124.

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