Double K-shell Photoionization of Neon

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Introduction

Double photoionization of helium has been extensively studied as a probe of electron-electron interactions in the simplest case of a two-electron system [1-3]. Three manifestations of electron correlation are often discussed in theoretical treatments of double photoionization of helium and helium-like ions. First, "ground-state correlation" accounts for angular and radial correlation between the two equivalent 1s electrons in the ground state. Second, "shake off" occurs when one of the electrons is photoejected, and the sudden change in screening of the nuclear charge can result in ejection shake off of the second electron. Third, in "knockout," the photoexcited electron can undergo a binary collision with the second electron, and both get ejected. The same electron-electron interactions are expected to govern double K-shell photoionization in higher-Z atoms, with the energy variations of double-K photoionization cross sections following Z-scaling laws [4]. In the high-energy limit, the double-to-single K-shell photoionization cross-sectional ratio R can be accurately calculated for helium and helium-like ions, because electron-electron interaction in the final state is negligible and only ground-state correlation is needed. Accurate $1s^2$ ground-state wave functions can be constructed, and the Z dependence of R in the asymptotic limit can be calculated [5, 6]. At lower energies, R depends on dynamic correlation in the final state (i.e., the knockout interaction). Measurements of R as functions of Z and of photon energy are needed to test and develop the theory and our understanding of electron correlation in inner-shell ionization processes.

Since K-shell electrons are localized near the nucleus and are more tightly bound than electrons in outer subshells, their interactions with outer electrons can be neglected to a first approximation. Double K-shell photoionization measurements on high-Z atoms can therefore be compared with calculations on helium-like ions of the same Z. The intense, tunable x-ray beams provided at the APS are well-suited for these measurements. We have measured R for the neon atom (Z = 10) at 5000-eV photon energy, where the knockout interaction is expected to be strong, and we have made comparisons with high-energy-limit calculations [5, 6] and an empirical Z-scaling law [7]. A full report on this study is in Ref. 8.

Methods and Materials

For atoms beyond helium, double K-shell photoionization cannot be determined unambiguously from ion charge-state yields. For neon, we used Auger-electron spectroscopy to record the KK–KLL hypersatellites that result when double-K vacancy states are produced. The single-K ionization energy of neon is 870.21 eV, and the double-K ionization energy is 1863 eV. Measurements were made on the 12-ID undulator beamline at the APS, with the x-ray energy tuned to 5000 eV. The x-ray beam passed through a neon gas jet, and a cylindrical-mirror electron analyzer recorded the emitted Auger electrons. The Auger-electron spectrum plotted in Fig. 1 is dominated by the K–$L_{2,3}L_{2,3}$ ^1S and

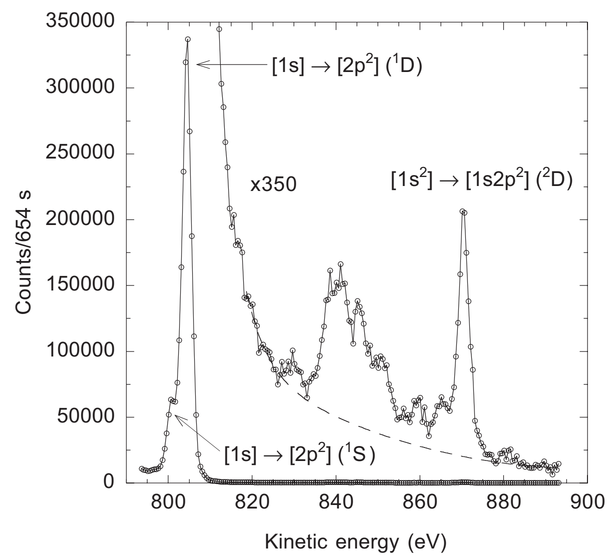

FIG. 1. Auger electron spectrum of neon excited by absorption of 5000-eV x-rays. The K–$L_{2,3}L_{2,3}$ ^1S and ^1D diagram lines and the KK–$KL_{2,3}L_{2,3}$ ^2D hypersatellite line are indicated. The structure between 830 and 860 eV is discussed in the text. The dashed curve beneath the peaks in the 820- to 890-eV region is the estimated background and tail of the diagram peaks.

[1]D diagram lines near 805-eV kinetic energy that result from single-K vacancies. The KK–$KL_{2,3}L_{2,3}$ ^2D hypersatellite line at 870.5 eV that results from double-K vacancies is also observed on an expanded scale. The position and width of the hypersatellite peak agree well with multiconfiguration Dirac-Fock (MCDF) calculations [9]. The structure between 830 and 860 eV is complicated by contributions from several multivacancy states, apparently including L-shell ionization in addition to double K-shell ionization. Additional vacancy states that are likely to be produced were identified by using shake calculations, and their Auger spectra were calculated by using the MCDF method and compared with the measured spectrum [8].

Results and Discussion

The double-to-single K-shell photoionization cross-sectional ratio R was determined from the relative intensities of the K–$L_{2,3}L_{2,3}$ ^1D diagram line and the KK–$KL_{2,3}L_{2,3}$ ^2D hypersatellite line, along with branching ratios into the respective final states from single-K and double-K vacancies taken from other experiments and theory. Our measured result R = 0.32 ±0.04% for neon is plotted in Fig. 2, along with measurements on helium at high energy (5.4 to 9.1 keV) [10] and at 190 eV [1], where the R value for helium reaches its maximum. The measurements are compared with the high-energy-limit calculations for helium-like systems [5]. While the high-energy measurement on helium agrees with the calculated asymptotic ratio, the helium measurement at 190 eV is larger by a factor of ≈2, and the present result for neon at 5000 eV is larger than the calculated ratio by a factor of ≈4. The experimental R values for higher-Z atoms determined from intensity ratios of x-ray fluorescence hypersatellites to diagram lines are also larger than the high-energy-limit calculations [7]. In these cases and for neon at 5000 eV and helium at 190 eV, the photon energies used are within the broad maximum of the double-K photoionization cross section calculated by Z scaling [4], where knockout is an important interaction. An empirical Z-scaling law was determined in Ref. 7 by fitting R values measured at energies where knockout is important, including the helium measurement at 190 eV. This empirical curve is plotted in Fig. 2 and gives R = 0.28 ±0.03% for neon, in good agreement with the measurement. A comparison of the empirical and asymptotic curves in Fig. 2 thus gives a rough estimate of the effect of knockout relative to shakeoff plus ground-state correlation. The knockout interaction appears to increase in relative importance as Z increases. We have also recently studied double K-shell photoionization of silver (Z = 47) by recording x-ray fluorescence hypersatellites using an x-ray/x-ray coincidence method [11]. That work includes a comparison of measured, calculated, and empirical R values like those in Fig. 2 but extended to high Z.

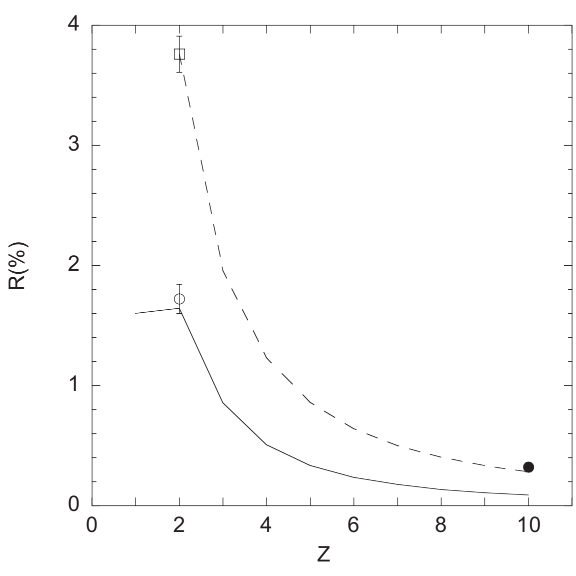

FIG. 2. Ratio of double-to-single K-shell photoionization cross sections measured for helium at 5.4 to 9.1 keV (open circle) [10], helium at 190 eV (open square) [1], and neon at 5 keV (closed circle) compared with results of high-energy-limit calculations on helium-like systems (solid curve) [5] and an empirical Z-scaling law (dashed curve) [7].

Acknowledgments

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