DOUBLE *K*-SHELL IONIZATION IN COLLISIONS OF FAST IONS WITH MID-Z ATOMS*

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K X-ray spectra from zirconium, niobium, molybdenum and paladium targets bombarded with 25 MeV/amu helium and 22.5 MeV/amu oxygen ions were measured using a high resolution transmission bent crystal spectrometer. Ratios of the double to single *K*-shell ionization cross sections were obtained from yields of the *K* hypersatellites and diagram lines. The results are compared to the semiclassical approximation predictions within the independent-particle model.

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High-resolution measurements of K X-ray spectra permit detailed studies of multiple inner-shell ionization processes and, in particular, of the double K-shell ionization. The multiple ionization induced by collisions with charged projectiles is generally assumed to result from uncorrelated single ionization processes. As a consequence, the probability of production of double K-shell vacancy states is equal in the first approximation to the square of the probability per electron to produce a single K-shell ionization. The radiative $K^{-2} \rightarrow K^{-1}L^{-1}$ transitions following the double K-shell ionization are called K hypersatellite X-rays. The ratios of double (σ_{KK}) to single (σ_K) K-shell ionization cross sections can be determined from the relative yields of resolved K hypersatellite X-rays. These cross section ratios offer a possibility to test the validity of theoretical models such as the independent particle semiclassical approximation (SCA).

The experiments were performed at the Paul Scherrer Institute in Villigen, Switzerland. ^{4}He and ^{16}O ions were accelerated to 25 MeV/amu and 22.5 MeV/amu, respectively, by the variable energy Philips Cyclotron. They were focused to a 1 mm wide and 20 mm high beam spot corresponding to the dimensions of the targets. Self-supporting metallic targets of natural zirconium, niobium, molybdenum and palladium with thicknesses of 31.7 mg/cm^2, 9.1 mg/cm^2, 26.4 mg/cm^2 and 25.9 mg/cm^2, respectively, were used. The X-rays from the targets were measured with an online transmission crystal spectrometer in modified DuMond slit geometry [1,2]. In this geometry a 0.15 mm wide slit, placed on the focal circle between the target and the crystal, acts as the effective source of radiation (see Fig.1). The energy calibration of the spectra was based on the $K\alpha_1$ diagram lines measured on both sides of reflection. The beam current was monitored by measuring the target X-ray emission with a 0.5 cm^3 Si(Li) detector located behind the slit, below the target-to-crystal axis (see Fig. 1).

The profile of an X-ray line measured with a crystal spectrometer can generally be represented by a so called Voigt profile, which results from the convolution of a Lorentzian and a Gaussian. The Lorentzian represents the natural line shape of the X-ray transition, the Gaussian corresponds to the instrumental response of the spectrometer broadened by the multiple ionization in the outer shells [3,4]. The natural line widths of the diagram lines were taken from Ref. [5], valid for singly ionized atoms, whereas the energies and intensities of these lines and widths of the Gaussian functions were used as free fitting parameters. The natural line widths of the hypersatellites were approximated by the method presented in Ref. [6]. The spectra were analyzed in the following way: first, the $K\alpha_1$ and $K\alpha_2$ diagram lines were fitted. The hypersatellite transitions were then analyzed using again Voigt profiles with energies, intensities and Gaussian widths as free parameters. Finally, yields obtained from the fitting procedure were corrected

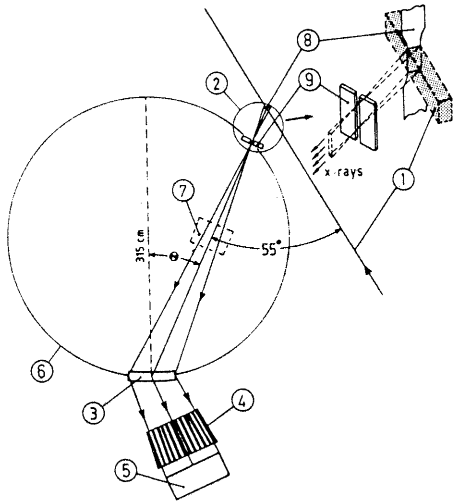

Fig. 1. Schematic diagram of the Du Mond slit geometry used in our experiments: (1) beam, (2) target chamber, (3) crystal, (4) colimator, (5) detector, (6) focal circle, (7) monitor detector, (8) target, (9) tantalum slit.

for the self-absorption of the observed X-rays in the target and their intensity attenuation by the crystal thickness. In K-shell ionizing collisions of heavy ions with atoms, the additional multiple M-shell ionization produces a broadening and energy shift of the X-ray lines. In our analysis we assumed that the broadening and energy shifts for diagram and hypersatellite lines were the same.

The double to single K-shell ionization cross section ratio can be expressed as:

$$\frac{\sigma_{KK}}{\sigma_K} = \frac{w_K \sum I(K^{-2} \to K^{-1}X^{-1})}{w_{KK} \sum I(K^{-1} \to X^{-1})}, \quad (1)$$

where w_{KK} and w_K are the fluorescence yields of doubly and singly K-shell ionized atoms, respectively, I stands for the intensity of the radiative transitions and X represents any possible subshell. If we assume that the K- and L-shell are ionized independently, the cross section for producing a highly excited state is given by the binomial distribution:

$$\sigma(K^{-2}L^{-n}) = 2\pi \int_0^\infty p_K^2(b) \begin{pmatrix} 8 \\ n \end{pmatrix} p_L^n(b)[1 - p_L(b)]^{8-n} b db, \quad (2)$$

where b is the impact parameter and p_K and p_L are the K- and L-shell ionization probabilities per electron. Considering only the most intense transitions and assuming $\omega_{KK} = \omega_K$, one can reduce Eq. (1) to:

$$\frac{\sigma_{KK}}{\sigma_K} = \frac{I(K\alpha_1^h)}{I(K\alpha_1)} \left(\frac{1 + \frac{I(K\alpha_2^h)}{I(K\alpha_1^h)}}{1 + \frac{I(K\alpha_2)}{I(K\alpha_1)}} \right) \left(\frac{1 + \frac{I(K\beta^h)}{I(K\alpha^h)}}{1 + \frac{I(K\beta)}{I(K\alpha)}} \right). \tag{3}$$

The intensity ratios $I(K\alpha_1^h)/I(K\alpha_1)$, $I(K\alpha_2^h)/I(K\alpha_1^h)$ and $I(K\alpha_2)/I(K\alpha_1)$ were extracted from the experiment and corrected for the different absorption in the target and crystal. Note that the intensity ratios $I(K\alpha_1^h)/I(K\alpha_2^h)$ generally differ largely from those of the diagram lines $I(K\alpha_1)/I(K\alpha_2)$ [6]. The last term in Eq. (3) can, to a good approximation, be put equal to one.

The theoretical single (σ_K) and double (σ_{KK}) cross sections for medium-mass atoms were calculated within the independent-particle approximation (SCA) for helium and oxygen projectiles, using hyperbolic classical trajectories and relativistic hydrogenic electronic wave functions. The results are presented in figure 2.

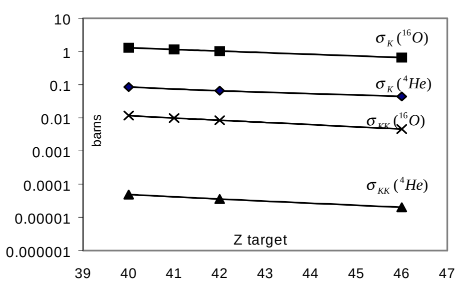

Fig. 2. Calculated single (σ_K) and double (σ_{KK}) K-shell ionization cross sections for ^{4}He (100 MeV) and ^{16}O (360 MeV) projectiles.

The experimental double to single K-shell ionization cross section ratios are compared with theoretical results in figure 3. The SCA theory, based on the independent-particle model, seems to overestimate the σ_{KK} cross section for collisions with 100 MeV α projectiles. On the other hand, the σ_{KK} values are underestimated for impact with 360 MeV ^{16}O ions, at least for the lighter targets.

The overestimation of σ_{KK} by theory for α particles can be explained by the fact that the second K-shell electron is ejected with a smaller probability than the first one as a result of increase of the electron binding energy following the removal of the first K-shell electron. This effect was not accounted for in the calculation. The underestimation of σ_{KK} by theory observed in the collision with oxygen ions may suggest that correlation effects are not negligible in the double K-shell ionization process with heavier projectiles.

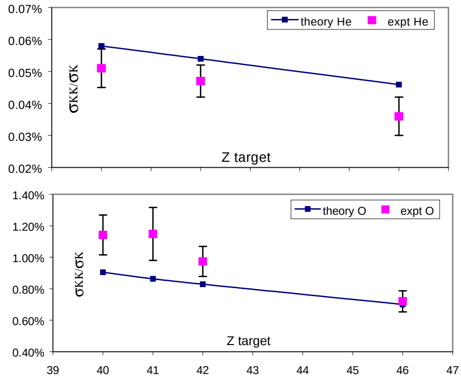

Fig. 3. Comparison between the measured and calculated σ_{KK}/σ_K ratios. The data for oxygen are from the present work, those for helium are from Ref. [6].

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