Photoionization of doubly charged scandium ions

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INTRODUCTION

Considering the fact that the ground state configuration of both neutral potassium and singly charged calcium is [Ar]4s, doubly charged scandium with its [Ar]3d ground state configuration is the simplest atomic system with an open 3d shell. It is even simpler than neutral scandium which in addition to the 3d electron has a closed $4s^2$ shell outside the argon core. Therefore photoionization (PI) of Sc^{2+} is fundamentally interesting, especially in view of the severe discrepancies between experimental [1] and theoretical [2] PI cross sections for neutral scandium in the region of 3p → 3d excitations. For these excitations PI of Sc^{2+} can be represented as

$$\begin{array}{lcl} h\nu + \mathrm{Sc}^{2+}(3s^2 3p^6 3d) & \rightarrow & \mathrm{Sc}^{2+}(3s^2 3p^5 3d^2) \\ & \searrow & \downarrow \\ & & \mathrm{Sc}^{3+}(3s^2 3p^6) + e^-. \end{array} \qquad (1)$$

Here the vertical arrow represents the intermediate doubly excited $3p^5 3d^2$ states decaying predominantly by autoionization via Super-Coster-Kronig transitions (vertical arrow), and the diagonal arrow represents the direct 3d PI channel. It is also possible to study the time reverse of Eq. 1, i. e. the photorecombination (PR) of a $Sc^{3+}(3p^6)$ ion with a free electron (e^-). Theoretically, on a state-to-state level, PI and PR cross sections are linked via the principle of detailed balance. It is evident that the study of both processes yields complementary information about the doubly excited intermediate states involved. Results of Sc^{3+} PR measurements, that have been conducted at the heavy-ion storage ring TSR of the Max-Planck-Institut für Kernphysik in Heidelberg, Germany, are already published [3]. Here, we report on first PI results obtained in August 2001 at the photon-ion research facility located at the ALS undulator beamline 10.0.1.

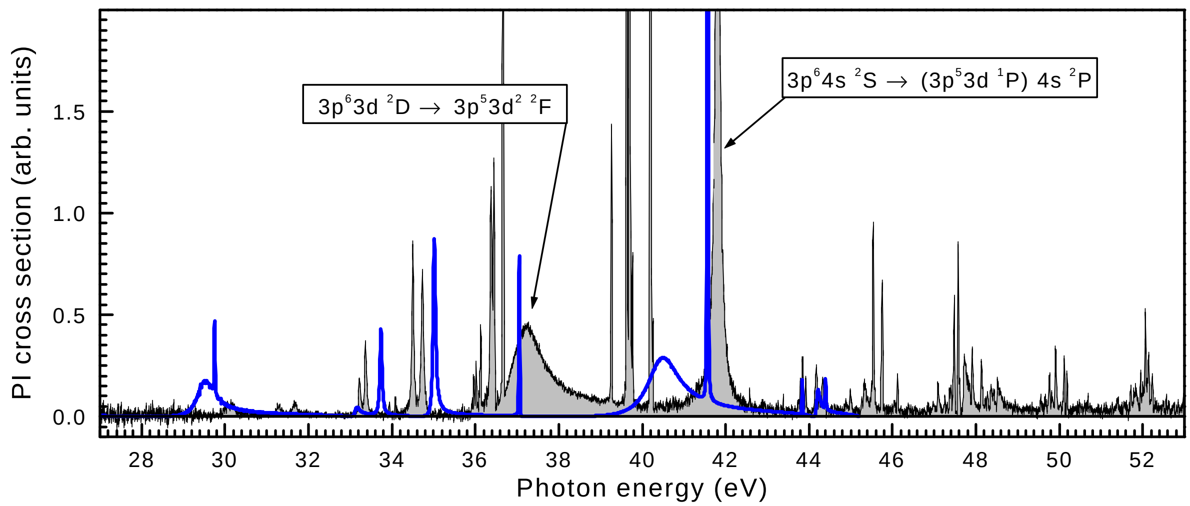

Figure 1: Part of the experimental spectrum (shaded curve) showing prominent resonances due to the excitation of the 3p^{6}3d ground state and of the 3p^{6}4s metastable state. The thick full line is the theoretical result of Altun and Manson [2].

EXPERIMENTAL PROCEDURE AND EXPERIMENTAL RESULTS

For the production of the Sc^{2+} ion beam, pieces of metallic scandium were vaporized inside an oven electrically heated to elevated temperatures. The Sc^{2+} ion beam was generated by ionizing the scandium atomic vapor by electron bombardment inside a compact electron cyclotron resonance (ECR) source. After having traveled through a bending dipole magnet serving for selecting the desired ratio of charge to mass, the ion beam was centered onto the counterpropagating monochromatized photon beam by applying appropriate voltages to several electrostatic ion beam steering devices. Electrical ion currents of up to 11 nA were available in the experiment. Behind the interaction zone the ion beam was deflected out of the photon beam direction by a second dipole magnet that also separates the ionized Sc^{3+} product ions from the Sc^{2+} parent ions. The Sc^{3+} ions were counted with nearly 100% efficiency with a single particle detector. From the measured Sc^{3+} count rate the PI cross section is readily derived by normalization on both photon flux and ion current.

The experimental photon energy range 23–68 eV encompasses the direct 3d and 3p photoionization thresholds. The experimental photo-ion spectrum is dominated by autoionizing resonances due to 3p excitations predominantly decaying via Coster-Kronig and Super-Coster-Kronig transitions (Fig. 1). The identification of the resonances is difficult. Only the most prominent resonance features can be identified with the aid of atomic structure calculations. The accurate calculation of resonance energies, widths and strengths for atomic systems with open 3d shells is a challenging task. The highly correlated nature especially of the doubly excited 3p^{5}3d^2 states requires large basis set expansions. Nevertheless, calculated resonance positions deviate by up to 3 eV from the measured resonance energies (Fig. 1).

Figure 2 shows resonances occuring in the energy range 36.62-36.72 eV. The exper-

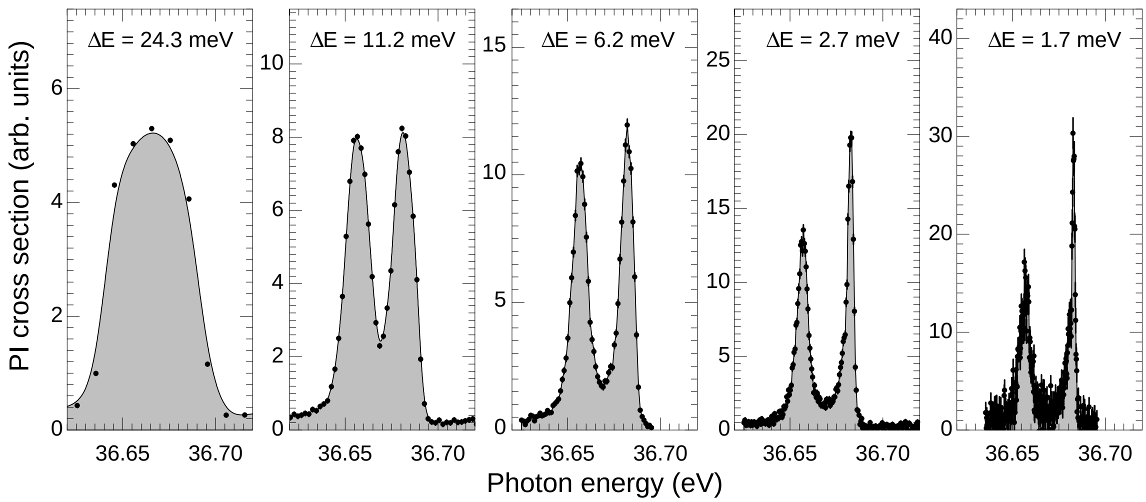

Figure 2: Influence of the experimental resolution on the measured photoionization cross section for a group of 3 resonances located around 36.67 eV.

imental photon energy spread was adjusted in a range of approximately 24 meV down to 1.7 meV by changing the width of the exit slit of the monochromator. At the highest resolution three individual resonances become visible. Likewise individual resonances located around $E \approx 40.2$ eV have been measured with an instrumental energy spread ΔE as low as 1.16 meV corresponding to a resolving power of $E/(\Delta E) \approx 35\,000$.

One complication with multiply charged ion beams extracted from an ECR ion source is the existence of a usually unknown amount of metastable ions in the beam. In the measured PI spectrum of Sc^{2+} (Fig. 1) we have identified resonances due to PI of the $Sc^{2+}(3p^6 3d\,^2D_{3/2})$ ground state as well as resonances due to PI of the $Sc^{2+}(3p^6 3d\,^2D_{5/2})$ and $Sc^{2+}(3p^6 4s\,^2S_{1/2})$ metastable states. A novel possibility to extract the fractions of metastable ions is provided by the comparison of the measured PI cross sections with the experimental PR cross sections of Schippers et al. [3] via detailed balance. The work is still in progress.

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