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Multiple Capture Contributions In Charge Exchange Induced X-ray Spectra And Their Relevance To Astrophysical Applications

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Abstract. In this work, we present theoretical line emission cross sections for Ar^{18+} and Ne^{10+} colliding on Ar for impact energies in the range 5 eV/amu-10 keV/amu which covers typical EBIT-traps as well as Solar Wind energies. The present analysis is performed by means of a 5-body classical trajectory Monte Carlo (CTMC) model which allows us to model the multiple capture contribution to the X-ray line emission spectra. Our results are contrasted to recent capture and line emission data from Berlin-EBIT, NIST and the University of Nevada Reno.

Keywords: X-ray emission, charge exchange, multiple capture.
PACS: 34.70.+e, 32.30.Rj, 32.70.Fw, 95.30.Ky

INTRODUCTION

During the last few years, many efforts were devoted towards a better understanding of line emission cross sections which follow charge exchange processes between highly charged ions and different atomic and molecular species. This interest has been strongly influenced by the fortuitous discovery of the cometary X-ray emission by the German satellite ROSAT in 1996 [1,2]. Although many different mechanisms were initially proposed to describe the X-ray emission, the data provided by ROSAT had low resolution (about 300eV) that didn't give any further clue on its physical origin. It was only a few years later, in the year 2000, and after the Chandra X-ray Observatory was put in orbit and produced X-ray images of an improved resolution of about 100eV, that the charge exchange mechanism was finally recognized as the major contributor to the cometary X-ray emission. Astrophysicists soon realized, with the information at hand, that all the ingredients needed to predict such emission were available since 1968: the properties of the cometary coma, the solar wind velocity and its heavy ion content, the average cross sections of charge transfer reaction (at the total cross section level, not state-selective) and the energies released in the subsequent recombination. A rough estimate for the X-ray luminosity of a comet in those days would have led 10^9 W, what would have easily identified comets as a new type of X-rays sources 30 years before ROSAT´s discovery [3].

In any case, soon after the discovery charge exchange was also found to be responsible for X-ray emissions originating in planetary atmospheres as well as in the geocorona and the heliosphere. In recent years, search for evidence of charge-exchange induced X-ray emission from outside the heliosphere has taken place including as potential targets the interstellar medium, as well as stars and galaxies [4-6].

In view of the next generation of X-ray microcalorimeter spectrometers to be put in orbit in the ASTRO-H mission (4-7 eV resolution) or the International X-ray Observatory (2.5 eV resolution), high resolution data are expected to be collected in the next few years. Accurate line emission cross sections (theoretical and experimental from Earth-based laboratories) will then be needed in order to exploit the astrophysical data at their maximum.

Earth based-laboratories have carried on experiments based on linear accelerators together with Ge or SiLi detectors (JPL) [7,8], EBIT-traps (LLNL [9,10], NIST [11] and Berlin-EBIT [12]) and COLTRIMS devices together with Ge detectors (UNR) [13]. Collision chambers with extraction lines have the drawback that photons arising from transitions involving metastable states like $O^{6+}(2^3S)$

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(lifetime ~10^{-3}s) might not be collected due to the typical extraction lines length. At solar wind energies, the ion would travel a distance of 400-700 m before the photon is emitted. EBIT-traps circumvent this issue but typical collision energies are about two orders of magnitude below the Solar Wind energy range of about 1 keV/amu. In this sense, an exact replica of the astrophysical conditions is still out of reach at Earth-based laboratories.

From the theoretical side, on the other hand, most of the published studies were performed within the multi-crossing Landau-Zenner (MCLZ) model [14,15], the classical overbarrier model (COB) [16] (which inherently provides *n*-state selective cross sections but for which *l*-state distributions should be included ad-hoc) and the classical trajectory Monte Carlo (CTMC) [17-19]. For the latter, the (*n*,*l*)-distributions are inherently provided by the method. At low impact energies, low *l*-values are mainly populated leading to spectra consisting of several Ly lines. At large impact energies the statistical distribution is reached, for which most of the emission is concentrated in the Ly-α line. At intermediate energies these two scenarios are smoothly merged although a natural propensity has been established towards the statistical *l*-distribution.

The resolution of the typical Ge detectors (130eV-160eV) operational at Earth-based laboratories highlights an important and challenging point and that is how the multiple capture contribution to the X-ray spectra is accounted for in the theoretical models.

THEORETICAL METHOD

In our 5-body CTMC model the classical evolution of a projectile + three electron-target is studied by numerically solving the Hamilton´s equations via a Runge-Kutta algorithm of adaptive step size. The three electrons are sorted with sequential binding energies over the quantum mechanical momentum distributions corresponding to the Ar(3p), Ar^{+}(3p) and the Ar^{2+}(3p) states for which we use the Clementi-Roetti expansions [20]. Coulomb potentials with individual effective charges set in order to provide the best possible agreement with the quantum mechanical radial distributions are employed for the electron-target interactions.

Multiple capture is treated in this context as follows: double capture events to levels n_1 and n_2 for which $|n_2-n_1|\leq 1$ are assumed to lead to autoionizing double capture,

$$\begin{aligned} Ar^{18+} + Ar &\rightarrow Ar^{16+*}(n_1 l_1, n_2 l_2) + Ar^{2+} \\ &\rightarrow Ar^{17+*}(nl) + e + Ar^{2+} \\ &\rightarrow Ar^{17+}(1s) + h\nu_1 + e + Ar^{2+} \end{aligned} \quad (1)$$

The electron with the greater n_c is considered to autoionize with zero energy. Conserving energy, the inner electron falls to a deeper *n* value and its *l* value is modified by preserving the orbital eccentricity.

Events for which $|n_2-n_1|>1$ are treated as double radiative decay and the decay routes of both electrons are explicitly considered,

$$\begin{aligned} Ar^{18+} + Ar &\rightarrow Ar^{16+*}(n_1 l_1, n_2 l_2) + Ar^{2+} \\ &\rightarrow Ar^{16+}(1s^2) + h\nu_1 + h\nu_2 + Ar^{2+} \end{aligned} \quad (2)$$

As a distinctive feature, we notice that the successive decay of both electrons lead to a shoulder located on the low energy side of the dominant Ar^{17+}(2p 1s) transition.

For three electron capture, we noticed that most of our events correspond to two electrons capture with nearly equal *n* values while the third one is bound to a deeper *n´* value. The following scheme has been assumed: the two outer electrons autoionize with zero energy while the third one falls to a deeper *n* level preserving its orbital eccentricity:

$$\begin{aligned} Ar^{18+} + Ar &\rightarrow Ar^{15+*}(n_1 l_1, n_2 l_2, n_3 l_3) + Ar^{3+} \\ &\rightarrow Ar^{17+*}(nl) + e_1 + e_2 + Ar^{3+} \\ &\rightarrow Ar^{17+}(1s) + h\nu_1 + e_1 + e_2 + Ar^{3+} \end{aligned} \quad (3)$$

In all cases the line emission cross sections have been calculated as in ref. [18].

RESULTS

In Figure 1 we benchmark our theoretical results with the data obtained by Ali *et al* [13] at the University of Nevada Reno for the single capture channel (SCX) in 4.54 keV/amu Ne^{10+} + Ar collisions by using a COLTRIMS device including two position-sensitive-detectors. From their analysis, relative *n*-state selective cross sections are obtained by fitting their energy gain or Q-value spectrum. The CTMC results shown have been convoluted by means of Gaussian functions for which we have set the FWHM in 12eV, a value at which we found the best agreement with the energy widths of the data. . Nevertheless, we note that the present experimental spectrum exhibits a shoulder

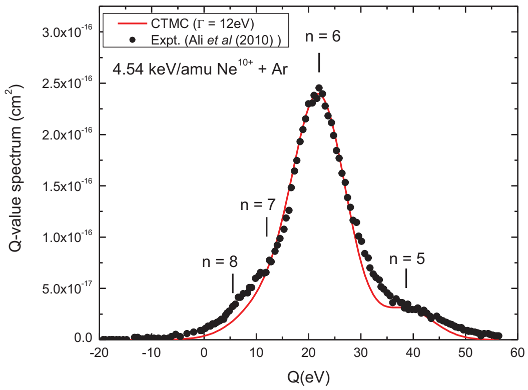

FIGURE 1. (Color online) Q-value spectrum for the SCX channel in 4.54 keV/amu Ne^{10+} collisions on Ar. The relative experimental data of Ali *et al* (ref. [13]) are normalized to the CTMC results (solid line).

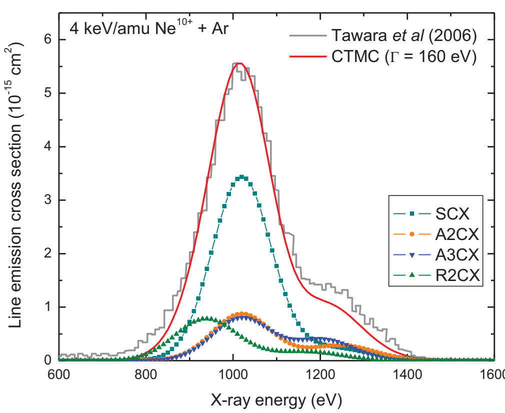

FIGURE 2. (Color online) Line emission cross sections for 4 keV/amu Ne^{10+} collisions on Ar. The theoretical separate contributions of the multiple capture channels are explicitly shown. The corresponding legends are SCX: single capture; A2CX: autoionizing double capture; A3CX: autoionizing triple capture and R2CX: radiative double capture. Experimental data are those from NIST as published by Tawara *et al.* (ref. [11]) and are normalized to the CTMC results.

in the region associated to electron capture to n = 8 which is not reproduced by our theoretical results.

In Figure 2, our CTMC line emission cross sections are compared to the NIST data for 4 keV/amu Ne^{10+} +Ar as published by Tawara *et al* [11]. In their study, these authors employed the EBIT-trap as an ion source and performed the collision process in a separate chamber (i.e. extraction mode). The separate theoretical contributions of the SCX and the different multiple capture channels are explicitly shown. From our treatment, it can be seen that autoionizing double and triple capture mainly enhance the higher Ly lines, while double radiative decay gives rise to the typical shoulder found at lower energies of the Ly-α peak. Although the reported resolution is of 130 eV at 4.50keV, at the present emission energies (600eV-1400eV) we had to increase the resolution to 160eV in our theoretical convolution procedure in order to properly reproduce the data.

In Figure 3, we show similar data for 4 keV/amu Ar^{18+} +Ar collisions. Again the agreement obtained with the data is very good and clearly highlights the low energy shoulder on the Ly-α peak which we ascribe to radiative double decay. In this case we used the reported FWHM of 130 eV in the theoretical convolution procedure.

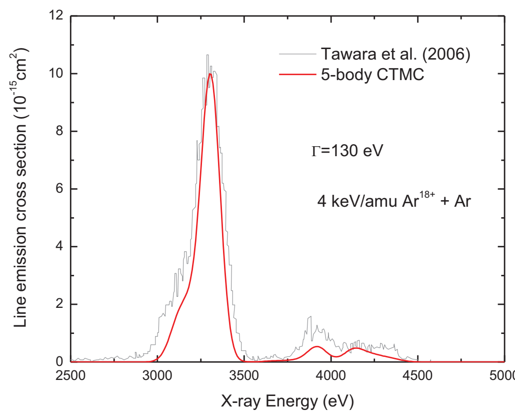

FIGURE 3. (Color online) Thin solid line: line emission cross sections for 4 keV/amu Ar^{18+} collisions on Ar. Experimental data are from Tawara *et al.* (ref. [11]). Thick solid line: present CTMC results. The experimental data are normalized to the CTMC results.

Finally in Figure 4 we show line emission cross sections for 18 eV/amu Ar^{18+} +Ar collisions performed with the Berlin-EBIT in both extraction and magnetic trapping modes [12]. In their analysis, Allen *et al* [12] showed that at typical EBIT energies their magnetic trapping results are in agreement with those from LLNL [9, 10] while at Solar Wind energies their results are in agreement with the extracted beam results from NIST [11]. Clear discrepancies among these two techniques are evident from the experimental spectra shown which were collected at the same nominal collision energy. We notice that the present CTMC results are in agreement with the extraction mode results. Further attempts to reconcile the two sets of data by theoretical exploration included sensitivity tests on the collision energy and the existence of possible electric fields in the trap. However, those explorations did not clarify the differing experimental results. In the magnetic trapping mode, in order to isolate the Ar^{17+} spectrum from those arising from other charge states of Ar, in particular that of Ar^{16+}, the corresponding spectra are manually subtracted. It is then not clear how the contribution coming from radiative double capture by Ar^{18+} is accounted for in the magnetic trapping mode, since those photons would be associated to the final Ar^{16+} ionic state. This suggests that events corresponding to radiative double capture should be present in the extraction mode spectra but not in the magnetic trapping mode, leading for the latter a larger relative contribution arising from the higher Ly-lines.

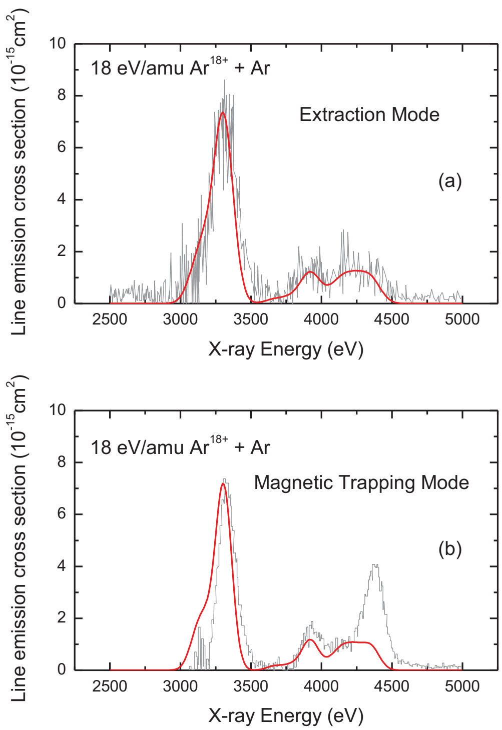

FIGURE 4. (Color online) Thin solid line: line emission cross sections for 18 eV/amu Ar^{18+} collisions on Ar obtained with Berlin-EBIT in the extraction mode (a) and the magnetic trapping mode (b) (ref. [12]). Thick solid line: present CTMC results. The experimental data are normalized to the CTMC results.

CONCLUSIONS

In view of the recent experimental advances in terms of microcalorimeter spectrometers and the planned missions to put more sophisticated X-ray observatories in orbit, the need of accurate line emission cross sections (either theoretical or experimental) is imperative.

We have introduced a 5-body CTMC model which allows for an explicit modeling of the multiple capture contribution to the charge exchange X-ray spectra. This contribution has been so far, and at best, grossly estimated for certain collision systems. A full description and understanding of the multiple capture contribution for different collision systems of interest is still out of reach.

We have showed that our line emission cross sections are in very good agreement with line emission cross sections from Berlin-EBIT and NIST, both obtained with EBIT-traps in the extraction mode.

More data for these collision systems would be welcome, in particular concerning the magnetic trapping mode-extraction mode discrepancies which so far have remained elusive from the experimental side. Such major differences present a large uncertainty if EBIT cross sections are used to de-convolute astrophysical data.

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