X-ray signatures of charge exchange in L-shell iron and sulfur

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Abstract. The X-ray signatures of L-shell charge exchange in sulfur and iron were studied in the laboratory. Charge states from S$_{11}^+$ to S$_{14}^+$ and Fe$_{18}^+$ to Fe$_{24}^+$ were created in electron beam ion traps (EBITs) and were left to interact via charge exchange with neutral gases. The measurements were monitored with a high-resolution microcalorimeter spectrometer for sulfur and a moderate-resolution SiLi solid-state detector for iron. Comparison of the charge exchange (CX) spectra with those obtained under electron-impact excitation showed marked differences. In particular, we show that CX shifts the centroid energy of the dominant $n = 3 \to n = 2$ emission. We explain this by an enhancement of the intensity of the 3s $\to$ 2p transitions and a shift towards lower energy of the 3d $\to$ 2p peak.

1. Introduction

Laboratory L-shell charge exchange (CX) emission data are important for understanding CX as an X-ray production mechanism. CX emission has proven to be of great importance in the solar wind interaction with both cometary comae and planetary atmospheres [1]. However, X-ray emission from CX is poorly understood. Assumptions made in the early X-ray emission models of the K-shell CX emission were shown to be inadequate when compared to laboratory data [2]. Even more updated, sophisticated models [3, 4, 5, 6] can still not fully reproduce many of the important features in K-shell CX emission [7].

L-shell CX emission is even harder to model than K-shell CX emission, and less laboratory data exist. Only EUV emission from low-Z ions (C, N, O) [8, 9, 10] and some X-ray spectra from high-Z ions (Kr, U) [11, 12] have been measured. Laboratory data of L-shell CX are essential in order to guide the development of theory [13].

We here present two recent measurements of L-shell CX emission: moderate-resolution results from the L-shell iron ions, Fe$_{17}^+$ to Fe$_{23}^+$; and high-resolution results from the L-shell sulfur ions, S$_{10}^{10+}$ to S$_{13}^{13+}$.

2. Experimental setup

CX emission from L-shell iron was created on EBIT-II [14] at the Livermore EBIT facility. The sulfur CX measurements were performed on SuperEBIT [14], also at Livermore. The highly
charged ions were produced, excited and trapped using the electron-trapping mode [15]. When the charge-state equilibria had been reached, the beam was turned off and the ions could CX with neutral gas in the magnetic-trapping mode [15]. A typical timing pattern for CX, which was used in the iron measurement, is shown in Fig. 1. In the iron measurement the neutral targets were background gases in EBIT, such as O\(_2\), N\(_2\), H\(_2\)O, and CO\(_2\) [16]. In the sulfur measurement, most of the CX reactions were with neutral SF\(_6\) gas, which was continuously leaked into the trap. However, there is always background gases present in the trap and there could also be some molecular fragments of SF\(_6\). These gases could act as neutral targets in the CX reactions and there is no way for us to distinguish whether the CX is with SF\(_6\) or with background gases. The iron and sulfur measurements, respectively, were monitored with a moderate-resolution SiLi solid-state detector (resolving power E/∆E \(\approx\) 10, at around 2 keV) [16] and a high-resolution microcalorimeter spectrometer (resolving power E/∆E \(\approx\) 80, at around 400 eV) [17]. The interacting iron ions Fe\(^{18+}\) to Fe\(^{24+}\) were produced at electron beam energies between 1.65 keV and 2.45 keV and the sulfur ions S\(^{11+}\) to S\(^{14+}\) were produced at 3.09 keV.

![Figure 1. Experimental timing sequence for the L-shell iron measurement.](image)

3. Measurement of iron L-shell charge exchange

In the electron-impact excitation spectra, the strongest feature is the peak due to the \(n = 3 \rightarrow n = 2\) transitions. At electron beam energies of 1.65 keV and 1.85 keV, this peak can be observed at 990 eV and 1025 eV, respectively. The corresponding energies for the \(n = 4 \rightarrow n = 2\) peak are 1290 eV and 1380 eV, respectively. Also the \(n = 5 \rightarrow n = 2\) peak is visible but is significantly weaker than the \(n = 4 \rightarrow n = 2\) peak.

Whereas for direct excitation the peak intensity decreases as a function of \(n\), CX shows a different pattern. The intensity observed with the SiLi detector at the location of the \(n = 4 \rightarrow n = 2\) transitions is strongly enhanced compared to the \(n = 3 \rightarrow n = 2\) peak. The \(n = 5 \rightarrow n = 2\) peak is of similar intensity as the \(n = 4 \rightarrow n = 2\) peak, and hence shows an even greater enhancement. The unresolved CX emission from the levels of electron captures, \(n_c = 8-10 \rightarrow n = 2\), can also be observed. This peak is weaker than the \(n = 5 \rightarrow n = 2\) peak, showing a similar or lower enhancement. Fig. 2 shows the electron-impact excitation spectrum overlaid with the CX spectrum. The peak around 0.5 keV is due to oxygen, which is one of the background gases in EBIT [16]. The factors of enhancement in CX is about 2 for the \(n = 4 \rightarrow n = 2\) peak, ranges between 3 and 4 for the \(n = 5 \rightarrow n = 2\) peak and ranges between 2 and 4 for the \(n_c = 8-10 \rightarrow n = 2\) peak [16].

Fig. 3 shows an overlaid direct excitation spectrum with a CX spectrum, where the \(n = 3 \rightarrow n = 2\) emissions of both spectra are normalized to each other and the oxygen peak, that was visible in figure 2, has been subtracted. The enhancement in the flux from \(n \geq 4\) is clearly visible. However, it is also observable that the \(n = 3 \rightarrow n = 2\) peak is slightly shifted towards lower energy in CX. Unfortunately, the charge states are only roughly the same in the two overlaid spectra [16]. However, if this shift is significant, it would suggest that the transition 3s...
→ 2p has been enhanced in the CX spectrum, as it has the lowest energy of the $n = 3 \rightarrow n = 2$ transitions [16].

![Figure 2. Overlaid Fe X-ray spectra from direct excitation with charge exchange at electron beam energy 1.85 keV.](image1.png)

![Figure 3. Comparison of Fe X-ray spectra produced by direct excitation at electron beam energies 1.75 keV in direct excitation and 1.85 keV in CX. The oxygen peak has been subtracted.](image2.png)

4. Measurement of sulfur L-shell charge exchange

In the L-shell sulfur CX spectra the individual transitions in the $n = 3 \rightarrow n = 2$ peak can be observed due to the significantly improved resolution of the micro-calorimeter [17]. The results are, in fact, the first high-resolution data of L-shell CX, with a resolution just below 5eV in the measurement. As a result, we can investigate the potential change in the $n = 3 \rightarrow n = 2$ peak, as intimated by the iron data. We will here focus mainly on the lithium-like lines, even though lines from lower charge states are present in the spectra.

In the direct excitation spectra, we see a similar pattern as in the iron measurement. The spectrum is dominated by the $n = 3 \rightarrow n = 2$ transitions; for S XIV that is 3d $\rightarrow$ 2p, 3p $\rightarrow$ 2s and 3s $\rightarrow$ 2p in order of decreasing intensity. These lines were found between 369 eV and 407 eV, as shown in Fig. 4. This is an overlaid spectrum of the $n = 3 \rightarrow n = 2$ transitions of lithium-like sulfur in direct excitation and CX, where the respective 3d $\rightarrow$ 2p peaks have been normalized to each other. A significant change in these transitions is the enhancement in the 3s $\rightarrow$ 2p peak in CX, as well as enhancement in the 3p $\rightarrow$ 2s peak. In addition, the 3d $\rightarrow$ 2p peak, which is however blended with lower charge states, also shifts to lower energy. Since the 3s $\rightarrow$ 2p peak has the lowest energy of the $n = 3 \rightarrow n = 2$ transitions, and the 3d $\rightarrow$ 2p shifts towards lower energy, this means that the centroid of the $n = 3 \rightarrow n = 2$ emission shifts to lower energy when produced by CX. This observation agrees with the centroid shift intimated by our iron measurements.

5. Discussion and summary

The principal quantum number of the electron capture can be approximated by the Janev and Winter approximation [18]. For iron ions ($q \leq 24$) this gives $n_c \approx 8$-10. This agrees quite well with the experimental data. For helium-like sulfur ($q = 14$) reacting with SF$_6$, the approximation gives $n_c \approx 8$. This agrees with what we observe in the spectra from the sulfur measurement (full analysis in progress).
We have detected a shift in the \( n = 3 \rightarrow n = 2 \) centroid energy during the CX excitation of iron. It seems plausible, if this shift is significant, that the 3s→2p transition has been enhanced in CX. In the high-resolution results from lithium-like sulfur, Fig. 4, this specific enhancement is actually resolved. In addition, the blended 3d-2p peak shifts to lower energy. This suggests that the \( n = 3 \rightarrow n = 2 \) centroid energy shift, in CX, might be an L-shell CX feature.

For L-shell ions, an electron captured into a level \( n_c \) can only decay to the 2s or 2p states if it is captured in an angular momentum state s, p, or d due to the \( \Delta l = 1 \) selection rule which governs the electric dipole transitions. For charge transfer to higher l-states the electron typically cascades down by a series of transitions, changing its l-value with 1 for every step [7]. The enhanced emission from \( n = 4 \) and 5 could either be populated by a single electron capture into \( n_c \), followed by cascades to \( n = 4 \) and 5, or by multi-electron capture where one electron drops from the capture level while the second electron autoionizes. Which of these paths the electron takes depends among other things on the collision energy of the electron. Low collision energy favors low l-state capture [19]. Since we observe a strong enhancement of the high-\( n \) flux, we may assume that low l-levels were populated in the charge transfer, which suggests that low-l double electron capture is more probable than high-l capture into \( n_c \) followed by cascades. Hopefully, detailed radiative cascade models will someday be able to discern which of these processes is more probable [16].

Acknowledgments
Part of this work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported in part by NASA grants to LLNL, SAO, UC Berkeley and GSFC as well as by LLNL Laboratory Directed Research and Development project OG-ERD-010.

References
[1] Bhardwaj A, Elsner R F, Randall Gladstone G, Cravens T E, Lisse C M, Dennerl K, Branduardi-Raymont G, Wargelin B J, Hunter Waite J, Robertson I, stgaard N, Beiersdorfer P, Snowden Steven L and Kharchenko V 2007 Planetary and Space Science. 55 1135–1189
[2] Beiersdorfer P, Behar E, Boyce K R, Brown G V, Chen H, Gendreau K C, Graf A, Ga M F, Harris C L, Kahn S M, Kelley R L, Lepton J K, May M J, Neill P A, Pinnington E H, Porter F S, Smith A J, Stahle C K, Szynkowiak A E, Tillotson A, Thorn D B, Trabert E and Wargelin B J 2003 Nuclear Instruments and Methods in Physics Research Section B 205 L99–L102
[3] Kharchenko and Dalgarno 2001 The Astrophysical Journal 554 173–177
[4] Perez J A and Olson R E 2005 Nuclear Instruments and Methods in Physics Research Section B 241 134–138
[5] Kharchenko V, Rigazio M, Dalgarno A and Krasnopolsky V A 2003 The Astrophysical Journal 585 L73–L75
[6] Otranto S, Olson R E and Beiersdorfer P 2006 Physical Review A 73(2)
[7] Wargelin B J, Beiersdorfer P, Neill P A, Olson R E and Scofield J H 2005 The Astrophysical Journal 634 687–697
[8] Bliek F W, Woestenenk G R, Hoekstra R and Morgenstern R 1998 Physical Review A (Atomic, Molecular, and Optical Physics) 57 221–226
[9] Lubinski G, Juhsz Z, Morgenstern R and Hoekstra R 2000 Journal of Physics B: Atomic, Molecular, and Optical Physics 33 5275–5296
[10] Lubinski G, Juhsz Z, Morgenstern R and Hoekstra R 2001 Physical Review Letters 86 616–619
[11] Beiersdorfer P, Olsen R, Schweikhard L, Liebisch P, Brown G, Crespo Lopez-Urrutia J, Harris C, Neill P, Utter S and Widmann K 2000 CP500, The physics of Electron and Atomic Collisions., published by American Institute of Physics, Melville, NY, 2000, edited by Itikawa, Y et al.
[12] Tawara H, Richard P, Siftonova U I, Vasilyev A A, Hansen S and Shlyaptseva A S 2002 Physical Review A 65(4)
[13] Wargelin B J, Beiersdorfer P and Brown G V 2008 Canadian Journal of Physics 86 151–169
[14] Beiersdorfer P 2008 Canadian Journal of Physics 86 1–10
[15] Beiersdorfer P, Schweikhard L, Crespo López-Urrutia J and Widmann K 1996 Review of Scientific Instruments 67 3818–3826
[16] Beiersdorfer P, Schweikhard L, Liebisch P and Brown G V 2008 The Astrophysical Journal. 672 726–732
[17] Porter F S, Beck B R, Beiersdorfer P, Boyce K R, Brown G V, Chen H, Gygax J, Kahn S M, Kelley R L, Kilbourne C A, Magee E and Thorn D B 2008 Canadian Journal of Physics 86 231–240
[18] Janev R K and Winter H 1985 Physics Reports 117 265–387
[19] Ryufuku H and Watanabe T 1979 Physical Review A 20 1828–1837