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CRITICAL TEST OF SIMULATIONS OF CHARGE-EXCHANGE-INDUCED X-RAY EMISSION IN THE SOLAR SYSTEM

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ABSTRACT

Experimental and theoretical state-selective X-ray spectra resulting from single-electron capture in charge exchange (CX) collisions of Ne^{10+} with He, Ne, and Ar are presented for a collision velocity of 933 km s^{-1} (4.54 keV $nucleon^{-1}$), comparable to the highest velocity components of the fast solar wind. The experimental spectra were obtained by detecting scattered projectiles, target recoil ions, and X-rays in coincidence; with simultaneous determination of the recoil ion momenta. Use and interpretation of these spectra are free from the complications of non-coincident total X-ray measurements that do not differentiate between the primary reaction channels. The spectra offer the opportunity to critically test the ability of CX theories to describe such interactions at the quantum orbital angular momentum level of the final projectile ion. To this end, new classical trajectory Monte Carlo calculations are compared here with the measurements. The current work demonstrates that modeling of cometary, heliospheric, planetary, and laboratory X-ray emission based on approximate state-selective CX models may result in erroneous conclusions and deductions of relevant parameters.

Key words: atomic data – atomic processes – comets: general – solar wind – X-rays: general

1. INTRODUCTION

X-ray and extreme-ultraviolet (EUV) emission has been detected from more than 20 comets since the first observation by Lisse et al. (1996). The charge exchange (CX) mechanism between highly charged solar wind (SW) minor heavy ions and cometary neutrals suggested by Cravens (1997) is now recognized as the primary process responsible for the observed emission (see, e.g., Lisse et al. 2001; Krasnopolsky & Mumma 2001; Krasnopolsky et al. 2002; Beiersdorfer et al. 2003; Kharchenko et al. 2003; Willingale et al. 2006; Bodewits et al. 2007; Lisse et al. 2007, and references therein). In the solar wind charge exchange (SWCX) mechanism, electrons are captured from cometary neutrals by SW ions into excited states of the product ions, which may then decay radiatively and in the process emit X-ray radiation. The SWCX mechanism has been invoked with various degrees of sophistication to model and interpret cometary X-ray and EUV emission spectra (Häberli et al. 1997; Wegmann et al. 1998; Schwadron & Cravens 2000; Kharchenko et al. 2003; Otranto et al. 2007) and has been the subject of numerous reviews (Cravens 2002; Krasnopolsky et al. 2004; Bhardwaj et al. 2007; Dennerl 2008). It has been argued that cometary X-rays represent a potential tool to monitor not only cometary activity, but also the composition, velocity, and flux of the SW in regions that spacecraft cannot reach (Cravens 1997; Dennerl et al. 1997; Schwadron & Cravens 2000; Beiersdorfer et al. 2001).

It is now also recognized that heliospheric X-ray emission due to SWCX with H and He interstellar neutrals (see, e.g., Cox 1998; Cravens 2000; Pepino et al. 2004; Robertson et al. 2009, and references therein), and X-ray generation throughout the terrestrial magnetosheath due to SWCX with geocoronal neutrals (see, e.g., Dennerl et al. 1997; Cox 1998; Cravens et al. 2009, and references therein), contribute to the soft X-ray background (SXRB). SWCX with H and O has also been proposed to account for the first definite detection of X-ray emission from the exosphere of Mars (Dennerl et al. 2006).

Understanding and accurately predicting these and related phenomena require novel experiments which simultaneously measure detailed (i.e., charge and quantum state resolved) collision parameters in coincidence with consequent atomic energy de-excitation to elucidate the underlying chain of mechanisms in this CX-induced X-ray emission, and ultimately, development of theoretical methods capable of broadly treating such interactions. To this end, several experimental groups have carried out laboratory studies of relevant collision systems (see, e.g., Beiersdorfer et al. 2000, 2001, 2003; Greenwood et al. 2001; Hasan et al. 2001; Gao & Kwong 2004; Ali et al. 2005; Bodewits et al. 2006; Mawhorter et al. 2007; Allen et al. 2008; Djurić et al. 2008, and references therein). Of particular importance for accurate modeling is the ability to predict the $n\ell$-state-selective CX cross sections (i.e., to account for the distributions of the principal n and angular momentum ℓ quantum numbers of the product projectile ions). All previous modeling attempts to simulate cometary or heliospheric X-ray spectra (Häberli et al. 1997; Wegmann et al. 1998; Rigazio et al. 2002; Beiersdorfer et al. 2003; Kharchenko et al. 2003; Otranto et al. 2007; Otranto & Olson 2008) have adopted simple $n\ell$ empirical relations, scalings from related collision systems, or fits to laboratory non-coincident total X-ray spectra. It should be noted, however, that non-coincident laboratory spectra contain contributions from a variety of reaction channels such as single-electron capture (SEC) and autoionizing and non-autoionizing multiple-electron capture (MEC). A superposition of several reaction channels is also likely to occur in cometary, planetary, and heliospheric spectra. Therefore, a technique which is capable of differentiating between the primary reaction channels is required for the interpretation of such spectra.

In this Letter, we report an experimental investigation of the n-state-selective hydrogen-like ion X-ray spectra following SEC in collisions of Ne^{10+} with He, Ne, and Ar neutral targets at a laboratory frame collision velocity v of 933 km s^{-1} (4.54 keV $nucleon^{-1}$). This velocity is at the upper end of the SW ion velocities. The present interactions are close analogs of the interactions of heavy minor, multiply charged, SW ions with cometary, planetary, and heliospheric neutrals. Specifically, the dominantly molecular constituents of cometary and planetary atmospheres (e.g., H_2O, CO_2) are simulated by gases of similar ionization potential and multielectron character (i.e., Ar, Ne). Helium, being the second most abundant (15%) interstellar neutral (Koutroumpa et al. 2009), is of direct relevance to heliospheric X-ray emission. The present spectra are free from complications arising from the inability of previously employed non-coincident total X-ray spectra to differentiate between the primary reaction channels. Consequently, they offer the opportunity to test critically the ability of theories to describe SWCX interactions at the $n\ell$ quantum level.

2. EXPERIMENT

Simultaneous cold-target recoil ion momentum spectroscopy (COLTRIMS) and X-ray spectroscopy were used for the triple-coincident detection of X-rays, scattered projectiles, and target recoil ions. COLTRIMS has been reviewed by Dörner et al. (2000), while the components of the experimental apparatus have been described elsewhere (Hasan et al. 1999; Ali et al. 2005). Briefly, the $^{22}Ne^{10+}$ ions were provided by the University of Nevada, Reno, 14 GHz electron cyclotron resonance ion source, and guided to the collision chamber where they crossed supersonic target jets at 90°. The target recoil ions resulting from the collisions were extracted by an electric field, at 90° relative to the incident ions and jet, and detected by a position-sensitive detector (PSD). The scattered projectile ions were charge analyzed electrostatically and detected by another PSD where their impact positions provided their final charge states, while coincident time-of-flight (TOF) measurements between projectile and recoil ions provided the recoil ion charge states. X-rays emitted at 90° relative to the incident ions were detected by a windowless high-purity germanium detector, placed opposite to the recoil detector. Coincidences between projectile ions and X-rays ensured that all detected particles originated in the same collision event. The full width at half-maximum (FWHM) of the X-ray peaks is energy-dependent with a value of about 126 eV for the Ne^{9+} Lyα line (1021.8 eV) and ∼133 eV for the Lyδ line (1307.7 eV).

3. RESULTS, THEORY, AND DISCUSSION

Since no electrons are directly ejected to the continuum for the considered collision energy, the change in electronic energy of the collision system, or the Q-value, is a direct measure of the projectile state population immediately following the collision. Q-value spectra, therefore, provide the experimental n-state-selective relative cross sections σ_n^{rel}. The Q-value for SEC is given by $Q \approx -(P_\parallel v + v^2/2)$ (Ali et al. 1992), where $P_\parallel$ is the longitudinal (i.e., parallel to the incident projectile direction) momentum transfer to the recoiling target. $P_\parallel$ of the recoil ions were determined from their TOF and impact positions on the PSD. Figure 1 displays the Q-value spectra for pure SEC for the three considered collision systems with the σ_n^{rel} indicated. These spectra were obtained using COLTRIMS-only measurements to acquire sufficient statistics for the accurate determination of σ_n^{rel}.

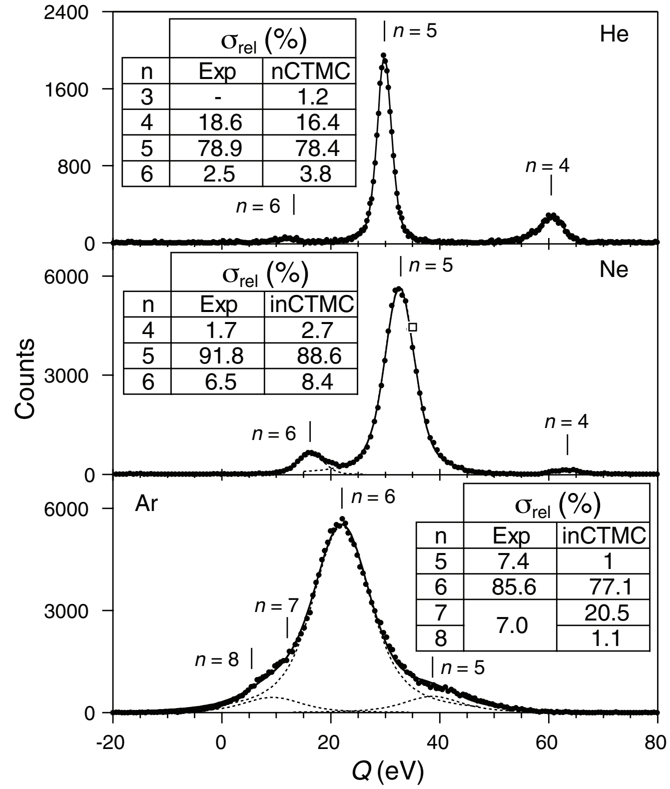

Figure 1. Experimental SEC Q-value spectra for collisions of 933 km s^{-1} $^{22}Ne^{10+}$ with He, Ne, and Ar targets. Both experimental and theoretical n-state-selective relative cross sections σ_n^{rel} are tabulated for each target.

Non-perturbative quantum-mechanical treatments of highly charged ion collisions with multielectron targets are difficult. A recent study of Cl^{7+} collisions with H (Zhao et al. 2007) demonstrates that such calculations are not routine, but require particular care, significant computational resources, and individual consideration. Therefore, we adopt a more tractable approach to model the measured interactions: the well-established classical trajectory Monte Carlo (CTMC) method (Olson & Salop 1977). The basic CTMC approach for bare ion collisions involving single-valence electron targets was discussed in Hasan et al. (2001), while elaborations for multielectron targets in the context of total MEC was given in Ali et al. (2005). The He target was treated using the former method with the electron–nuclear charge interaction described by an effective charge $Z_{\mathrm{eff}} = 1.6875$, designated as nCTMC (i.e., "CTMC" for "n" electrons bound by the atom's sequential ionization potentials). For the Ne and Ar targets, six valence electrons within the independent particle model were considered (inCTMC). The electron–atomic core interaction was treated with a model potential. The standard microcanonical ensemble for the initial electron orbitals was filtered to remove all but the p orbitals.

Examination of the experimental and CTMC σ_n^{rel} displayed in Figure 1 clearly shows that the agreement is excellent for both the He and Ne targets and reasonable for Ar. Reasonable agreement between experiment and CTMC has been reported previously by Cassimi et al. (1996) for Ne^{10+} and Ar^{18+} on He at a slightly higher collision velocity (≈1143 km s^{-1}). That reasonable success has prompted the use of CTMC $\sigma_{n\ell}$ to simulate non-coincident total cometary and laboratory X-ray spectra (Otranto et al. 2007; Otranto & Olson 2008) under the assumption that the spectra are dominated by SEC. As we previously demonstrated (Ali et al. 2005), these spectra

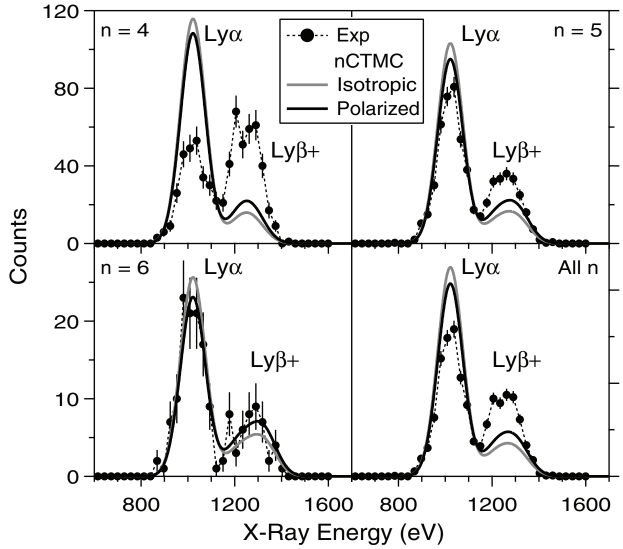

Figure 2. Experimental and CTMC modeled n-state-selective and overall H-like Ne^{9+} X-ray spectra following SEC by Ne^{10+} from He. The modeled spectra assume isotropic emission (gray solid line) and maximum polarization for Lyβ+ emission (black solid line). The theoretical and experimental areas are normalized to each other to facilitate comparison. The overall spectra preserve the experimental and theoretical σ_n^{rel}.

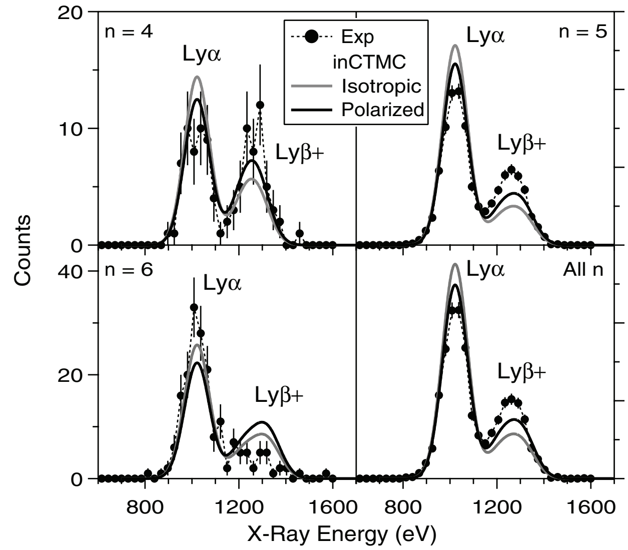

Figure 3. Same as in Figure 2 but for SEC from Ne.

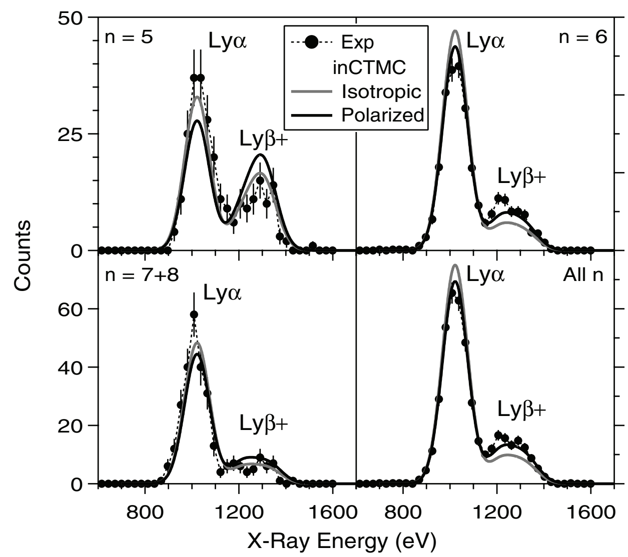

Figure 4. Same as in Figure 2 but for SEC from Ar.

may contain significant contributions from MEC. Furthermore, very high resolution (FWHM $\approx$ 10 eV) total X-ray spectra using an X-ray microcalorimeter show clear signatures of MEC (Beiersdorfer et al. 2003). These and similar signatures in later work could not be accounted for by other SEC CTMC calculations (Otranto et al. 2007), and the relative contributions to certain high-energy emission lines from SEC and MEC remain in question (Wargelin et al. 2005, 2008). Total X-ray spectra are, therefore, not the appropriate benchmarks for testing the validity of theoretical CX methods for simulating X-ray spectra.

A major advantage of the simultaneous COLTRIMS and X-ray spectroscopic measurements is that it is not only possible to separate X-rays originating in pure SEC from those due to MEC (Ali et al. 2005), but it is also possible to obtain X-ray spectra corresponding to each populated n-level in the pure SEC channel as given in Figures 2–4. The present measurements also provide the opportunity to test the validity of the theoretical methods, such as CTMC, for X-ray spectra modeling by assessing their ability to predict $\sigma_{n\ell}^{\mathrm{rel}}$ for SEC, and therefore the ability to simulate the most direct and simplest of cases (i.e., n-state-selective X-ray spectra). To perform such a simulation, a radiative cascade model for the hydrogen-like Ne^{9+} ion was constructed giving the relative yields of the different Lyman X-ray lines starting from a certain initial $n\ell$-state. These yields, together with the CTMC $\sigma_{n\ell}^{\mathrm{rel}}$, the attenuation in the 300 Å copper contact layer of the X-ray detector, the variation of the FWHM of the Gaussian profiles with X-ray energy, and two X-ray radiation polarization scenarios, as explained below, have been taken into account in producing the CTMC n-state-selective X-ray spectra.

It is well known that X-ray emission following a CX collision is polarized (Vernhet et al. 1985). Since the polarization rates are unknown in the present work, we considered two extreme scenarios. The first assumes isotropic emission for all X-ray lines. This assumption enhances the relative intensity of the Lyα to the $n \geqslant 3 \rightarrow n = 1$ (Lyβ+) lines. The other scenario assumes isotropic emission for Lyα and adopts 100% polarization for the Lyβ+ emission that does not originate in or result from cascades passing through s-states. The latter scenario maximizes the intensity of the Lyβ+ lines relative to that of the Lyα line.

The CTMC modeled n-state-selective and overall H-like neon X-ray spectra following SEC by Ne^{10+} from the He, Ne, and Ar targets are shown in Figures 2, 3, and 4, respectively. The theoretical and experimental line areas are mutually normalized for comparison while the overall spectra preserve σ_n^{rel}. The CTMC spectra reveal a general underestimation of the population of low-ℓ states, which give rise to Lyβ+ lines, for the dominant n-level for each target. This is also reflected in the overall SEC X-ray spectra. For minor capture channels, the behavior is less systematic, though agreement appears to be the best with maximum polarization or for Ar targets. The present results, based on the best available practical theoretical model, demonstrate that it remains a significant challenge to simulate accurately even the most simple cases. Therefore, synthetic spectra of cometary, heliospheric, planetary, and laboratory total X-ray emission based on incompletely tested theoretical CX methods are not expected to be well founded. This complements results from earlier investigations which showed that the dominance of SEC assumed in the models is also not justified (Ali et al. 2005).

While the most recent X-ray emission simulations represent a major improvement over earlier efforts, which adopted equipartition or statistical angular momentum models (Häberli et al. 1997; Wegmann et al. 1998; Schwadron & Cravens 2000), the present results suggest that agreement with observations is likely to be fortuitous. Deductions of relevant parameters from such models should be considered as being associated with appreciable systematic uncertainties.

Considering the success of CTMC in accounting for $\sigma_n^{\rm rel}$ as shown in Figure 1, it may seem surprising that it underestimates the Lyβ+ intensity for the dominant n-levels. CTMC, however, has a propensity toward a more statistical ℓ-distribution (i.e., $\sigma_\ell \propto (2\ell + 1)$), at least for the lower ℓs. Further, the agreement is seen to improve with decreasing first ionization potential: He (24.6 eV), Ne (21.6 eV), and Ar (15.8 eV). In fact, the best agreement occurs for Ar which might be taken as a surrogate for the dominant species in cometary and planetary atmospheres responsible for the X-ray emission: H_2 (15.4 eV), CO (14.0 eV), CO_2 (13.7 eV), and H_2O (12.6 eV). The observation that the largest discrepancies occur for He suggests that the problem lies in electron-correlation effects which are known to be strongest for the He atom. Electron correlation is not sufficiently accounted for in the present CTMC calculations.

4. CONCLUSIONS

In summary, relative state-selective cross sections and X-ray spectra have been obtained from triple-coincident measurements of X-rays, scattered projectiles, and target recoil ions which provide a test of CX theories at the quantum orbital angular momentum level. While improvements in X-ray simulations based on CX models have been made, the current results show that agreement for the relative state-selective cross sections does not necessarily imply agreement for the state-selective X-ray spectra, and suggest that comparison of such models to observations of solar system X-rays may lead to faulty conclusions or parameter extractions.

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