X-RAY AND EUV SPECTROSCOPY OF VARIOUS ASTROPHYSICAL AND LABORATORY PLASMAS: COLLISIONAL, PHOTOIONIZATION AND CHARGE-EXCHANGE PLASMAS

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ABSTRACT

Several laboratory facilities were used to benchmark theoretical spectral models that are extensively used by astronomical communities. However, there are still many differences between astrophysical environments and laboratory miniatures that can be archived. Here we setup a spectral analysis system for astrophysical and laboratory plasmas to make a bridge between them, and we investigate the effects from non-thermal electrons and the contributions from a metastable level population on level populations and charge stage distribution for coronal-like, photoionized, and geocoronal plasmas. Test applications to laboratory measurement (i.e., electron beam ion trap plasma) and astrophysical observation (i.e., Comet, Cygnus X-3) are presented. A time evolution of the charge stage and level population are also explored for collisional and photoionized plasmas.

Key words: atomic processes – line: formation – plasmas – X-rays: general

Online-only material: color figures

1. INTRODUCTION

Since the launch of new-generation X-ray and EUV missions (e.g., Chandra, XMM-Newton, as well as Hinode and the Solar Dynamics Observatory (SDO) for solar physics), a large amount of high-quality spectra with high-resolution and imaging have posted deep insights for our understanding of universe objects, including their emission measurements, physical environment, space structure or morphology, heating mechanisms and so on (Güdel & Nazé 2009). Moreover various spectral models were constructed for the understanding of the observational data, such as Chianti (Landi et al. 2012), MEKAL (Mewe et al. 1995), AtomDB (Smith et al. 2001), Cloudy (Ferland et al. 1998), Xstar (Kallman & Bautista 2001), and so on. However, they are strongly dependent on the data accuracy of underlying atomic processes. So a different branch of astrophysical research—Laboratory Astrophysics (LA)—appears to benchmark these theoretical models of celestial emissions (Foord et al. 2004; Fournier et al. 2001) or to simulate the astrophysical phenomenon in a morphology directly based upon some scaling method, such as jets, shocks, and magnetic reconnection (Zhong et al. 2010), etc. (see the review by Remington et al. 2006 for details).

An electron beam ion trap (EBIT) was usually used to benchmark various spectral models for electron collision plasmas or to help line identification for coronal-like plasmas due to its characteristics of dissociation of various atomic processes (González-Martínez et al. 2006) and of consistent plasma condition (via the electron density ranging from 10⁹ to 10¹³ cm⁻³) to astrophysical cases (Liang et al. 2009). Yet, EBIT runs generally on monoenergetic electron beams, which differs from the astrophysical cases with thermal electrons. Furthermore, polarization effects from unidirectional beams play an important role on line intensity of energetic electron beams, which differs from the astrophysical cases (Liang et al. 2009). Moreover various spectral models were posted deep insights for our understanding of universe objects, including their emission measurements, physical environment, space structure or morphology, heating mechanisms and so on (Güdel & Nazé 2009). Moreover various spectral models were constructed for the understanding of the observational data, such as Chianti (Landi et al. 2012), MEKAL (Mewe et al. 1995), AtomDB (Smith et al. 2001), Cloudy (Ferland et al. 1998), Xstar (Kallman & Bautista 2001), and so on. However, they are strongly dependent on the data accuracy of underlying atomic processes. So a different branch of astrophysical research—Laboratory Astrophysics (LA)—appears to benchmark these theoretical models of celestial emissions (Foord et al. 2004; Fournier et al. 2001) or to simulate the astrophysical phenomenon in a morphology directly based upon some scaling method, such as jets, shocks, and magnetic reconnection (Zhong et al. 2010), etc. (see the review by Remington et al. 2006 for details).

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In this work, we present a description of an analysis package—Spectral Analysis System for Astrophysical and Laboratory (SASL) plasmas—for the spectroscopic measurements in a laboratory and its application to astrophysical observations. The theory and atomic data that are incorporated into this model are outlined in Section 2. Section 3 illustrates its applications for the spectroscopy of plasmas dominated by electron collision with thermal and monoenergetic (e.g., EBIT case) electrons and by photoionization (PI). Effects from non-equilibrium and metastable population on a level population and or charge stage distribution are examined for electron collision and photoionized plasmas. Moreover, the application of CX X-ray spectroscopy in comets is presented in this section. The last section gives a summary and conclusion.

2. THEORY AND ATOMIC DATA

An optically thin assumption is adopted in this model. The atomic model used to describe the line emission from a particular ionic species \((X^{q+})\) includes the upper level population due to electron/proton/photon impact (de-)excitation, electron/photon ionization from a lower neighbor ion \((X^{(q-1)+})\), dielectronic/radiative recombination (DR/RR) from a higher neighbor ion \((X^{(q+1)+})\), charge transfer in collisions with a neutral atom and molecule, and subsequence radiative decays, either directly to the ground and in lower excited states or via cascades, as shown in the following formula,

\[
\frac{dn_i^{q+}}{dt} = n_c \sum_{j \neq i} n_j^{q+} (Q_{ji}(T_e) + P_{ji}(T_e)) + \sum_{j > i} n_j^{q+} A_{ji} \tag{1}
\]
where \( n_i^{q+} \) is the number density of \( q+ \) charged ions at \( i \)th level state, while \( n_e \), \( \gamma \), and \( n_{mol} \) correspond to the number density of electrons, photons, and neutral atoms/molecules, respectively. \( Q_{ij} \) refers to the electron/proton impact (de-)excitation rate coefficient; \( P_{ij} \) corresponds to the photon (de-)excitation rate coefficient; and \( S_{ij} \) and \( \alpha_{ij} \) correspond to the electron impact ionization and dielectronic plus radiative recombination rate coefficients, respectively. \( \theta_{ij} \) and \( C_{ij} \) are PI and CX recombination rate coefficients, respectively. The first, second, and third terms in the right part of the equation correspond to contributions from electron/proton excitations and subsequent radiative decays. The terms of Equations (3) and (4) denote the contributions from electron impact ionization and dielectronic plus radiative recombination. The Equations (5) and (6) terms refer to population and depopulation due to PI and CX from neighbor ions. Furthermore, transitions among tens or hundreds of levels for each ion, and ionizations/recombinations to/from several/tens of levels of the neighbor ions have been assumed by consideration of data availability and practical applications. The above complex equation can be simplified to be

\[
d - \frac{N}{dt} = \Lambda N, \tag{7}
\]

where \( \Lambda \) is a stiff matrix that consists of parameters of various atomic processes mentioned above.

### 2.1. Level Energies, Radiative Decay Rates, and Excitations

Chianti version 7 (Landi et al. 2012) incorporates a large amount of data for ions with nuclear number from H to Zn from published atomic data, which is regarded as the most accurate, widespread and complete spectral model presently in wavelength range of 1–2000 Å by the solar/stellar community. So Chianti (ver. 7) database is the baseline data for the present model. For He-like (Whiteford et al. 2001), Li-like (Liang & Badnell 2011), B-like (Liang et al. 2012), F-like (Withotho et al. 2007), Ne-like (Liang & Badnell 2010), and Na-like (Liang et al. 2009a, 2009b) isoelectronic sequences from single ionized through up to krypton ions, as well as some astrophysical interested ions (Si \( \text{ix} - \text{Si xii} \), Liang et al. 2011; Li et al. 2013 and Fe \( \text{xiv} \), Liang et al. 2010), accurate calculations have been done within an intermediate close-coupling framework transformation or DARC R-matrix methods under the UK Rmax and APAP network,\(^3\) as well as LA project in China. So these data were used to update the level energies, radiative decay rates, and impact excitations data of charged H–Zn ions available from Chianti version 7. Here, those theoretical wavelengths were adjusted by using available NIST version \(^4\) level energies for some ions, e.g., N\(^{5+}\), O\(^{5+}\), Si\(^{3+}4+6+...12+\), Ar\(^{7+}8+...13+\), Ca\(^{10+}\), Fe\(^{16+}21+\), and Kr\(^{26+}31+\). An extension for ions up to krypton has been done for the above-mentioned iso-electronic sequences in this model. Moreover, the original effective collision strengths over large temperature ranges were used in the present SASAL, not scaled ones as done in Chianti model. This benefits the SASAL data update by direct replacement from data producers. Users do not need to do an onerous data scaling.

Yet the scaling procedure in Chianti extends its application to a more extensive temperature range than the present SASAL, that covers the limited temperatures that are available in the original effective collision strengths provided by the data producers. The storage of collision strengths in SASAL overcomes this limitation, which will be discussed again later. For He-like ions (Whiteford et al. 2001), 49 fine-structure (FS) level energies from 1s\(n\)l \((n = 1–5,l \in s, p, d, f, g)\) configurations, radiative decay rates, and impact excitations among these levels were incorporated into the SASAL model. For Li-like ions (Liang & Badnell 2011), valence- and core-electron excitations up to the 1s\(^2\)2\(l\) and 1s\(^1\)2\(l\) levels (total 204 FS levels) were included. For B-like ions (Liang et al. 2012), 204 close-coupling levels of the 2s\(^1\)2\(p\)^\((x + y = 3), 2s^2[3,4]l, 2s2p[3,4]l, and 2p\(^2\)3\(l\) configurations were included, and further radiative decay rates as well as impact excitation among them. For F-like ions (Withotho et al. 2007), 195-FS levels from 2s\(^2\)2\(^p\)^\(3\), 2s\(^2\)2\(p\)^\(2\)2\(s\), 2\(s\)2\(p\)^\(2\)4\(l\), and 2\(s\)2\(p\)^\(3\)5\(l\) configurations, radiative decay rates and impact excitations among these levels were included. For Ne-like ions (Liang & Badnell 2010), we included the data for 209-FS levels belonging to \(1s^22s^22p^5, 2s^22p^3[3,4]l, 2s2p^6[3,4]l, and 2p\(^2\)3\(l\) configurations. For Na-like ions (Liang et al. 2009a, 2009b), the data for 161-FS levels from 2s\(^2\)2\(p\)^\(3\)\(l\), 2s\(^2\)2\(p\)^\(3\)\(l\), \(2s2p^6, 6l\) \((l \in s, p, d, f, g)\) and 2s\(^2\)2\(p\)^\(6\)2\(l\) \((l \in s, p, d)\) configurations. For some astrophysical abundant ions \(\text{Si}^{8+} - \text{Si}^{12+}\), Liang et al. 2011; Li et al. 2013 and Fe\(^{13+}\), Liang et al. 2010), those data presented in literatures were incorporated into the SASAL database.

In order to analyze spectra due to excitations of non-thermal electrons, i.e., monoenergetic electrons in EBIT plasma, we store the original collision strength (see references above mentioned) as well, in addition to the effective collision strength for thermal electrons. But its large disk occupation makes the SASAL model to be not feasible for distribution because a large amount of data within the R-matrix framework have been incorporated. Then, we set the data to be offline with multiple averaging codes, e.g., Gaussian averaging for monoenergetic electrons and Maxwellian averaging for thermal electrons.

### 2.2. Dielectronic and Radiative Recombinations

State-of-the-art calculations for dielectronic and radiative recombination data have been performed by Badnell and coauthors (Badnell et al. 2003; Badnell 2006a) by using AUTOSTRUCTURE (Badnell 1986) for K-shell (Badnell 2006b;
Bautista & Badnell 2006), L-shell (Colgan et al. 2004, 2003; Altun et al. 2004; Zatsarinny et al. 2004a; Mitnik & Badnell 2004; Zatsarinny et al. 2003, 2006, 2004b), Na-like (Altun et al. 2006), Mg-like (Altun et al. 2007), and Al-like (Abdel-Naby et al. 2012) iso-electronic sequence ions from H through Zn, which were incorporated into the present model, including analysis fits for metastable levels and partial level-resolved recombination rates. For the partial level-resolved recombination rates, an automatic level-matching procedure was used to setup these data and match the level index to that of the above-mentioned level energies, where configuration, total angular momentum I, and energy ordering are taken to be a good quantum number (Liang et al. 2009b). These level-resolved dielectronic and radiative recombination rates significantly benefit the estimation of recombination emission lines in PI plasmas, which are stored as a separate data file for each ion. If the level numbers (ID$_{\text{P}}$) of recombined ion $X^{q\text{+}}$ stated in Section 2.1 are less than the level index of the recombined ion in the partial level-resolved data file, then those data recombined to levels above ID$_{\text{P}}$ are discarded directly by consideration of the lower population above one hundred or hundreds of levels. Such a simplified treatment might underestimate the recombination line emission for a specified transition due to cascades from higher levels. Their total rates are compiled separately by analysis fits for calculations of the charge stage distribution. For other M-shell ions, the available data from Chianti version 7 (Landi et al. 2012) were adopted here.

For He-like ions, dielectronic recombination satellite lines were implemented by using the following formulae (Gabriel 1972; Oelgoetz & Pradhan 2004)

$$i_s^{\text{DR}} = \frac{4\pi}{c^2} a_0^{3/2} X_{\text{He}} n_e T_e^{-3/2} \exp \left( -\frac{E_s}{kT_e} \right) g_s A' B^a ,$$

where $X_{\text{He}}$ is the ionic fraction of He-like ions in equilibrium and/or non-equilibrium, $B^a$ is the total autoionization branching ratio $\Sigma A'/(\Sigma A' + \Sigma A')$, $A'$ is the radiative decay rate, $a_0$ is the Bohr radius, $T_e$ is the plasma temperature, and $g_s$ and $A'$ are the transition energy and statistical weight of the upper level of a given satellite line, respectively. Those involved $E_s$, $A'$, and $A^a$ values are generated by an online flexible atomic code (FAC) program (Gu 2008) for Li-like ions via the calc_fac.pro program with an atomic model of [Li:] 1s$^2$[2/3/4]/l, 1s2s[2/3/4]/l, 1s2p$^2$, 1s2p[3/4]/l, and [He:] 1s$^2$, 1s[2/3/4]/l, 2s$^2$, 2s2p, 2p$^2$ configurations, where 1s$^2$2l configurations are used for optimization. For the dielectronic satellite spectra, Vainshtein & Safronova (1978, 1980) generated a large amount of data of the wavelengths, radiative transition probabilities, and autoionization rates for He-like ions with $Z = 4$–34. Because no electronic data available for their calculations, these data are not compiled into the SASAL at present, but it is in plan.

Radiative recombination continuum (RRC) is an important feature in the high-resolution spectroscopy of photoionized winds, i.e., Cygnus X-3 (Paerels et al. 2000). So we implemented such emissions into the present SASAL model. The RRC emissivity by this process is given as (Tucker & Gould 1966),

$$\frac{E}{dtdV d\omega} = \frac{dP}{dV dE_{\gamma}} = \frac{dP}{dV dE_{\gamma}} f(v_e) d\nu_e \frac{E_{\gamma} f(v_e) d\nu_e}{dE_{\gamma}^2} ,$$

where $E_{\gamma}$ is the photon energy of the recombination radiation, $\sigma_{\text{rec}}$ is the recombination cross section, and $f(v_e)$ denotes the distribution of the electron velocity in a plasma. By the Milne relation between PI ($\sigma_{\text{PI}}$) and the recombination cross section (Raymond & Smith 1977), as well as the Maxwell–Boltzmann distribution $f(v_e)$ for electron velocities, the above equation can be written as

$$\frac{dP}{dV dE_{\gamma}} = \frac{4\pi}{c^2} (2\pi m_e k T_e)^{3/2} n_e n_{(q+1)^+} E_{\gamma}^{3/2} \frac{g^{q+}}{g^{(q+1)^+}} \exp \left( -\frac{E_{\gamma}}{kT_e} \right) \sigma_{\text{PI,q+}}(E_{\gamma}),$$

where $g^{q+}$ is the statistical weight of a $q+$ charged ion. As shown by the above equation, the PI cross section is the fundamental parameter for the calculation of the RRC emissivity, so we store a high-resolution PI cross section from the data producers (e.g., Badnell group) for radiation calculations. In accessing the data of Verner et al. (1996), we slightly modified the “phfit2.f” program to be accessed by the IDL “spawn” command implicitly to obtain the PI cross section at different photon energies $E_{\gamma}$. The bin-size of photon energies depends on the line width that is selected for line emissions before the calculation. Here, we adopt the bin-size of $\Delta E_{\gamma} = (1/8)\lambda_{\text{FWHM}}$. In order to speed up the calculation for the charge stage distribution, especially for non-equilibrium photoionizing plasmas, we also store the PI rates with blackbody radiation at 23 temperatures over $10^{-3}$–1.0 keV. The PI data source will be explained in the next subsection.

### 2.3. Photoionization

For PI, the data from the compilation of Verner et al. (1996) were added into the present model, whose adopted analysis fits to the nonrelativistic calculations for the ground states of atoms and ions. Recent partial level-specific PI cross sections (Badnell 2006a; Witthoeft et al. 2009, 2011a, 2011b) were included systematically by an automatic level matching procedure in calculations as done for the above-mentioned level-resolved recombination rates, to account for contributions from a metastable level population. From H through Zn, the present model includes the cross sections from multi-configuration intermediate coupling distorted wave calculations (Badnell 2006a) for K- and L-shell PI as well as Na-like iso-electronic sequence ions. For several elements, such as Ne, Mg, Si, S, Ar, Ca, and Ni, it includes the latest Breit–Pauli R-matrix calculations (Witthoeft et al. 2009, 2011a, 2011b). For a few interested ions (e.g., carbon ions), R-matrix calculation performed by Nahar and coauthors (Nahar et al. 2000) were also included from the Web site maintained by them. The cross sections were extended up to infinity in the integration (i.e., blackbody radiation) by a tail from Kramer’s fit of $\sigma_{\text{PI}}(E) = 3 \text{sr} E_{\gamma}^3$. As mentioned in the above subsection for RRC emissivity calculations, a high-resolution PI cross section from the data producers are stored separately in the present SASAL model, which can be accessed in calculations. Although this makes it difficult to distribute the SASAL model to users, either the offline data access or specific data transfer for these high-resolution PI cross section is still possible. The final level-resolved PI cross section (Badnell 2006a; Witthoeft et al. 2009, 2011a, 2011b) including the K-shell vacancy benefits emissivity calculations.
for K-shell fluorescent lines as given by Kallman et al. (2004),

$$
\epsilon = E_\gamma \int_{E_{in}}^{\infty} F_{E_{in}} \sigma_K(E_\gamma) \frac{dE_\gamma}{E_\gamma} \omega_K n_{X} n_{q^+},
$$

where $n$ is the density of radiated plasma, $F_{E_{in}}$ is the local photon flux, $\omega_K$ is the fluorescent yield, $n_{X}$ refers to the X elemental abundance, and $n_{q^+}$ corresponds to its level population of photoionizing ions with a charge of $q+$ at jth stage. However, we have not compiled K-vacancy levels and relevant Auger and fluorescence yields (Gorczyca et al. 2003) for most L-, M-, and N-shell ions. So the present Sassal model cannot be used to analyze fluorescent lines. The present Sassal model is also not a self-consistent solution of level populations and radiative equilibrium for PI plasma, where level populations and ionization equilibrium are treated separately. In the treatment of the population of excited valence levels, only the population of the dielectronic recombination rates combines with the ground configuration of neighboring higher charged ions. Thus, it can be used for the analysis of discrete recombination lines in photoionized plasma. In the treatment of the ionization equilibrium, the total PI and dielectronic plus radiative recombination rates are used. A further explanation will be given in the corresponding subsection on applications.

### 2.4. Collisional Ionization

The total collision ionization cross section/rate with the excitation autoionization (EAI) contribution for some ions were given in Chianti version 7 (Landi et al. 2012). In order to investigate the effects due to metastable level population, we calculated the level-resolved ionization cross section by using FAC (Gu 2008) for He-like, L-shell, and Ne-like iso-electronic sequence ions from Li to Zn elements. The atomic model used for this calculation is given in Table 1, where the first configuration group (marked by an underline) is used to obtain the optimal radial potential. In the compilation and calculation of Dere (2007), there is no significant evidence of EAI contributions for He-like, B-like, C-like, N-like, O-like, and F-like ions. So we did not include EAI contributions for these iso-electronic ions. For Li-like ions, the EAI cross sections include excitations to the 1s22l’/1s2l2l’ and 1s2l2l’, and 1s2l2l’ levels. Here the EAI contributions are considered by using $\sigma_{EAI} = \sum_j \sigma_{exc}(j-k)B_0^{nl}$ (where $B_0^{nl}$ is autoionization branching ratio from the kth channel). For Be-like ions, the EAI cross sections include excitation to the levels of the 1s2l2p, 1s22l’/1s2l2l’, and 1s2l2l’ configurations. For Ne-like ions, the EAI cross sections via 2s2p63l and 2s2p64l levels are taken into account.

Because of recent interest on silicon in laboratory (Fujioka et al. 2009) and theory (Wang et al. 2011), as well as its diagnostic application in astrophysics (Milligan 2011), we select highly charged silicon ions (Si$^{q+}$—Si$^{11+}$) to examine the accuracy of the present FAC calculation (see Figure 1 for the total ionization cross section from the ground state of each ion). The cross sections were extended up to infinity for a parameterized formula for collision strength as given by Zhang & Sampson (1990) of $\Omega_{cl}(E) = B_0^{nl} n_{2l'} + p_{2l'} + p_{2l} \gamma/y + p_{2l} \gamma/y^2$, where $u = E/E_{in}$ and $y = 1–1/u$. In the following, we will briefly discuss the results one by one.

For Si$^{q+}$ ion, Thompson & Gregory (1994) concluded the presence of impurity metastable states to be 5% by comparing their measured data at incident electron energies of 50–100 eV with their prediction from the Lotz formula for the direction ionization (DI). However, significant discrepancies (∼17%: see Figure 2 in Thompson & Gregory 1994) between the measured and the Lotz cross section including the impurity of the metastable contributions were stated; this needs further elaborate calculations. The present FAC calculation confirms that the EAI contribution will enhance the ionization cross section more than ∼10–20% below $I_p$ ($I_p = 167$ eV) of scattered electron energy. When we tentatively assume the impure metastable (2p$^{5}$3s$^{3}$P) contribution of 10%, the present FAC calculation including the EAI contribution shows an excellent agreement with their measurement below the energy of ∼2$I_p = 334$ eV. Above this energy, the difference is also within 5% for most reported energies. The difference is less
Figure 1. Cross section of electron impact ionization for Si$^{4+}$–Si$^{11+}$ ions at their ground stages from different calculations and database along with available experimental data for Si$^{4+}$–Si$^{7+}$ ions.

(A color version of this figure is available in the online journal.)

than 1% between the present DI result and that in the Chianti compilation.

For Si$^{5+}$, fits to the measured cross sections (Thompson & Gregory 1994) were used in the Chianti version 7 compilation. The EAI contributions to the cross section are confirmed again to be disregarded. Because of the close energy split ($\sim 0.6$ eV) for the ground term $2s^22p^5{}^2P$, no apparent contribution from the metastable FS level ($2s^22p^5{}^2P^1/2$) was observed by Thompson & Gregory (1994). By assuming different fractions of impure metastable ions, the present FAC calculations demonstrate that the metastable contribution is negligible compared to the total ionization cross section, i.e., the 10% impurity fraction adopted in Figure 1.

For Si$^{6+}$, the present FAC calculations are lower than the experimental values by 20% (Zeijlmans van Emmichoven et al. 1993); however, the Lotz formula’s result and the Chianti version 7 compilation show better consistencies with the measurement within 10%. Zeijlmans van Emmichoven et al. (1993) suggested
technique, Fogle et al. (2008) derived a metastable (2$^1P^0$) that metastables of the 2$^1P^0$ levels can be negligible, for example 20% metastable fraction used in Figure 1.

For Si$^{14+}$, the present FAC calculation is lower than the Chianti version 7 compilation within 10%–15%. Yet it shows a better agreement with the experimental data within 10% (Zeijlmans van Emmichoven et al. 1993). For Si$^{8+}$, the present FAC calculations show a good agreement with the Chianti version 7 compilation within 10%.

For Si$^{10+}$, the present direct ionization cross section shows a good agreement with results of Dere (2007) within 10%. When the EAI contributions due to excitations to 1s2$^1P^0$, 1s2$^1P^0$3$^1S^o$, and 1s2$^1P^0$4$^1S^o$ were included, the resultant total cross sections will be enhanced by ~6% above scattered energy of 3$\lambda_p$ ($3\lambda_p = 476$ eV). Moreover, the autoionizations via 1s2$^1P^0$ levels are the dominant contribution to this enhancement. We further check other iso-electronic ions by comparison with available experimental data, e.g., O$^{14+}$ (Fogle et al. 2008) and Ne$^{5+}$ (Bannister 1996) as shown in Figure 2. For O$^{14+}$, the present DI cross sections are slightly higher than the experimental data at incident energies of 2$\lambda_p$–8$\lambda_p$ ($3\lambda_p = 114$ eV), but they are within 10%. At the threshold and high energy regions, the present results agree with the experimental measurement within uncertainty. The EAI contribution of 1s electron can be noticed above the incident energy of ~570 eV. Using the gas attenuation technique, Fogle et al. (2008) derived a metastable (2$\pi$2$^3P^0$) fraction of 0.24 ± 0.07 in their experimental ion beam. By assuming the same fraction of metastable impurity, we also calculate the total ionization cross section with the inclusion of EAI. The difference is within 15% between the total ionization cross section and the experimental measurement (Fogle et al. 2008). For Ne$^{5+}$, the EAI contribution is less than 5% above ~930 eV. The present DI+EAI calculations show a good agreement with the measurement by Bannister (1996) within experimental uncertainty except for a few energies. In view of the above discussion, the present DI+EAI calculation is reliable for Si$^{10+}$.

For Si$^{11+}$, the EAI cross section is confirmed to be less than ~1% of the total cross section. And the present results agree with the Chianti version 7 compilation within 10% below 1 keV. At energies of 1.0–3.0 keV, the difference between them is about 15%–20%. Above 3.0 keV, the difference becomes smaller again being less than 15%. For the simple case of He-like Si$^{12+}$, the present FAC results agree well with the Chianti version 7 compilation, and it is not presented in Figure 1 by consideration of page space.

By the above comparison, an uncertainty of 15% can be accepted for the present calculations of the collisional ionization. Then we expect the final accuracy to be within 15% for the Si ionization balance.

### 2.5. Charge Exchange Recombination

In order to obtain accurate CX cross sections in ion-atom/molecule (also, namely, “recipient-donor”) collisions, some sophisticated methods have been developed, including the molecular-orbital close-coupling method, the atomic-orbital close-coupling method, and the time-dependent density theory method. However, in many cases, the accurate charge transfer cross section data are very limited due to the difficulties in the sophisticated treatment of the complex systems, so the multichannel Landau–Zener (MCLZ) theory offers a flexible choice. Even in systems for which accurate calculations are possible, application of the Landau–Zener model can provide useful “first estimates” of non-adiabatic transition probabilities. Based on the two-state Landau–Zener model (Landau 1932; Zener 1932), the multichannel Landau–Zener theory with rotational coupling (MCLZRC) has been developed and was extensively used to estimate the cross section of multiple charged ions (“recipients”) with hydrogen and helium (“donors”) (Butler & Dalgarno 1980; Salop & Olson 1976; Janev et al. 1983). In MCLZRC model, electron transitions happen at the crossing regions $R_c$ of the potential curve of the collision systems and the transition probability $p_n$ can be estimated by the Landau–Zener formula, as given by

$$p_n = \exp \left( -\frac{\pi \Delta^2(R)}{2v_R \Delta F(R)} \right)_{R=R_c},$$  

where $R_n$ is the curve crossing position, $\Delta R$ is the energy splitting at the crossing point, $v_R = \sqrt{1 - \frac{b^2}{R_c^2}}$ is the radial velocity wherein $b$ is the impact parameter, and $\Delta F = (Z-1)/R_c^2$. In the case that the multi-state coupling dynamics can be reduced to a finite number of two-state close-coupling problems that are mutually isolated, the probability $p_n$ of a given exit $n$ will be populated within the quasi-classical approximation (Salop & Olson 1976). The original parameters of $R_n$ and $\Delta R$ can be computed by using accurate quantum chemical methods, for example, the multi-reference singly–doubly excited configuration interaction method. However, such quantum chemical methods are too expensive in computational time. Salop & Olson (1976) have proposed an approximation estimation method, in which the crossing point can be obtained based on the ionization energy of the “donor” and excitation energy of the recipient ion, and the energy splitting $\Delta R$ can be computed using the following analytical formula (within an accuracy of 17%)

$$\Delta(R_n) = 18.26 \sqrt{Z} \exp \left( -\frac{1.324 R_n}{\sqrt{Z}} \right).$$

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7 http://www-cfadc.phy.ornl.gov/xbeam/cross_sections.html
Using the parameterized MCLZRC model of Salop & Olson (1976), the CX cross section can be computed quickly, and we compile this parameterized MCLZRC code into the present model to estimate the CX cross section online for various “recipient” ions with donors, i.e., hydrogen and helium.

In the present version, only the parameterized MCLZRC code was compiled, and the original MCLZRC code is in planning due to complicated calculations for avoiding the crossing point and the adiabatic splitting energy. In this work, we first extract level energies of captured ions from the Sasa1 database, then obtain the averaged energy for each configuration nl or LS term. From these averaged energies and other necessary parameters (i.e., captured ion potential, donor potential and polarization, and exponent of a single orbital wave function), we can derive the avoided crossing point $R_n$ in this interaction, and the adiabatic energy splitting at $R_n$. Furthermore the nl-manifold CX cross section will be obtained. The resultant nl-manifold CX cross section is distributed to each level by statistical weighting. The whole calculation for selected ions can be done implicitly when the approximation is selected and not from compiled data from published papers or public Web sites.

In the following, we present the CX cross section of $\text{N}^+\text{A}^+$ colliding with H to check the reliability of this approximation. Figure 3 shows a comparison of the CX cross section between the present parameterized MCLZRC calculations and the previous quantum-mechanical molecular-orbital close-coupling (QMOCC) calculation (Wu et al. 2011) for the collision of the $\text{N}^+\text{A}^+$ ion with neutral H via n = 3, 4 channels. The original MCLZRC calculation (n = 4) shows an excellent consistency with the recommended data over the larger energy region, its realization of online calculations is in the plan. The figure also demonstrates that the present parameterized MCLZRC calculation is an acceptable choice for estimation of the CX contribution to the observed line emission. For solar wind velocities of ~200–800 km s\(^{-1}\) (~200–3500 ev u\(^{-1}\)), it shows a better agreement between the parameterized MCLZRC calculation and the recommended data from Wu et al. (2011). At lower recipient energies $E < 1.0$ keV, the donor electron prefers to transfer to $n = 4$ channel of the recipient ion, but this preference will shift to the $n = 3$ channel at higher energies of $E > 1.0$ keV. The widespread nature of such accuracy of the parameterized MCLZRC still needs further examination with elaborate calculations from the QMOCC or classical trajectory Monte Carlo (CTMC) methods for other ions. However, such data for astrophysical abundant ions are very scarce. Anyway, this comparison posts insights for the accuracy of the parameterized MCLZRC calculation. Moreover an energy-dependent CX cross section can be estimated, better than hydrogenic model, from which the solar wind dynamics can be estimated.

In collision with other donors, such as hydrogen gas (H\(_2\)), water (H\(_2\)O), carbon monoxide (CO), carbon dioxide (CO\(_2\)), and methane (CH\(_4\)), the polarizability (4.5) and exponent (−1.0) of the single orbital wave function for H was used for the estimation of CX cross section.

Furthermore, we complement the hydrogenic model that was adopted by Wegmann et al. (1997) into the present spectroscopic model to estimate the CX cross section, that is,

$$\sigma = 8.8 \times 10^{-17} \left( \frac{q - 1}{q^2/2n^2 - |l_p|} \right)^2,$$

where $q$ is the charge of the recipient ion, $n$ is the principal quantum number of captured ion with peak distribution at $n = q\sqrt{(1/(2|l_p|))}(1 + (q - 1)/\sqrt{2q})^{-1/2}$, and $|l_p|$ is the ionization potential of the donor in atomic units (i.e., 1 a.u. = 27.2 eV). The n-manifold cross section is distributed into the l-subshell according to the distribution function of $W(l, n) = ((2l + 1)((n - 1)!/n!)/((n - l - 1)!))$ for low $n \leq 8$ and of $W(l, n) = ((2l + 1)/n!)(n - l - 1)!^2$ for high $n > 8$ values. Finally, the level-resolved CX cross sections are obtained by the relative statistical weight of each level. The total n = 4 CX cross section $4.89 \times 10^{-16}$ cm\(^2\) is in agreement with the recommended data from Wu et al. (2011) (see the horizontal line in Figure 3).

Additionally, we compiled the CX cross section from the published literature. For example, the electron capture in collision between bared oxygen (O\(^{6}\)) and hydrogen [H(1s)], as performed by Shipsey et al. (1983), is compiled into the present model by weighting the l-sublevel cross section with the relative statistical weight of each level, in which the l-sublevel cross sections were derived from n-manifold cross sections $Q_n$ and the relative l-sublevel probabilities $P_l$ given in that work. The CTMC calculation performed by Otranto et al. (2007) and Otranto & Olson (2008) for the single electron capture of bare and hydrogenic recipients (carbon, oxygen, and neon) with water (H\(_2\)O) are also compiled into the present model with the same statistic weighting for the hydrogenic recipients as was done by them. The cross section of electron transfer in collisions of bared and hydrogenic carbon with hydrogen gas are from the OPEN-ADAS database. For the collision between hydrogen-like nitrogen (N\(^{6}\)) and atomic hydrogen, Wu et al. (2011) adopted QMOCC method, from which the recommended data for the LS term resolved over low- and high-energy regions are compiled into the present model.

In summary, both the parameterized MCLZRC and the hydrogenic methods are used in the present spectroscopic model to perform online calculations to obtain the CX cross section.
Figure 4. Theoretical spectra of Fe xiv at thermal (T_e = 2.0 MK) and modeled monoenergetic (E_e = 460 eV) electrons, along with measurement at Heidelberg EBIT facility (Liang et al. 2010).

(A color version of this figure is available in the online journal.)

3. APPLICATIONS AND DISCUSSIONS

We use the present SASAL model to analyze the X-ray and/or extreme ultraviolet spectroscopy in coronae-like, photoionized, and geocoronal astrophysical and/or laboratory plasmas.

3.1. Electron-collision Dominant Plasma

For the spectroscopy of thermal equilibrium, the present model is basically the same as that of Chianti version 7 (Landi et al. 2012) for those ions without a data update mentioned in Section 2.1 because that database is the baseline data in the present model. As explained in Section 2.1, new atomic structures and excitation data are incorporated for some ions, which will help new line identification and will improve spectroscopic diagnostic (see detail for Fe xiv spectroscopy in the work of Liang et al. 2010). Contributions of recombination and ionizations from/to neighboring ions can also be explored in the line emissions, in which the same procedure is adopted as in the discussion of the metastable effect in Section 3.1.2. Additionally, the original collision strengths are stored as offline data for non-thermal electron distributions due to its large requirement of disk size, whose origins are cited in Section 2.1 for the discussion of excitations. That is, users can setup any forms of electron energy distribution to avoid the invalidity problems of detail balance between the excitation rates and de-excitation rates for non-thermal electrons. In this work, we will pay attention to effects from non-thermal electrons (monoenergetic beam, e.g., EBIT plasma), metastable population, as well as their time dependence.

3.1.1. Non-thermal Effect

The electron beam ion trap (EBIT) has been regarded as a better choice to benchmark various theoretical models for coronal-like plasmas due to its electron density being consistent with astrophysical cases (Beiersdorfer 2003). However, it usually operates with monoenergetic electron beams, which will introduce non-negligible polarization as illustrated by Liang et al. (2009). So a direct comparison between the EBIT measurement and thermal prediction may have the potential problem as found in the work of Beiersdorfer & Lepson (2012). In Figure 4, we demonstrate the theoretical spectra of Fe xiv in a thermal plasma with a temperature of T_e = 2.0 MK, and in a modeled monoenergetic beam of 460 eV with a beam width of 30 eV at an electron density of 10^{10} cm^{-3}, along with the experimental measurement at the Heidelberg EBIT facility (Liang et al. 2010). For comparison, both the theoretical spectra are normalized to the experimental one at ~219.1 Å from the 3s^2 3d^2 D_{3/2} \rightarrow 3s^2 3p^2 P_{3/2} transition. For some weak emissions, their line intensities become lower than those in the case of thermal plasma, while some emissions become stronger. For example, weak emissions around 221.1 Å and 223.2 Å due to 3s3p3d^2 D \rightarrow 3s3p^2 P transitions, and lines around 216.6 Å and 216.9 Å due to 3s3p3d^2 D \rightarrow 3s3p^2 P transitions, becomes weaker in the modeled monoenergetic beam than those in the thermal plasma. In contrast, 3s3d^2 3D_{3/2} \rightarrow 3s3p^2 P_{1/2, 3/2} transition lines at 211.3 and 220.1 Å become stronger in monoeenergetic cases. The large difference between the measurement and theories results from the low density (10^{10} cm^{-3}) adopted here, and its density-sensitivity as demonstrated by Liang et al. (2010).

3.1.2. Time Evolution of Level Population and Ionic Fraction

During the impulsive phase of the solar flare, departures from the ionization equilibrium could occur (Del Zanna & Woods 2013). During the gradual phase, ionization equilibrium assumption is usually valid due to higher densities (Bradshaw & Cargill 2010). Milligan (2011) has pointed out that correlation between Doppler and non-thermal velocities during impulsive C-class flares are strongly dependent on the ionization equilibrium assumption. Smith & Hughes (2010) clearly shows the minimum and maximum timescales to the ionization equilibrium for each element from carbon through up to nickel over temperatures of 10^8–10^9 K.

Here by solving the time-dependent rate equation, we investigate the time evolution of a level population and ionic fraction. Figure 5(a) illustrates the time evolution of level population for the three lowest-lying levels (1s^2 2s^2 2p^3 P_{1/2, 3/2}) of Si^{8+} at an electron density of 10^{10} cm^{-3} and a modeled beam energy of 500 eV. Being less than n_e = 1.5 \times 10^9 cm^{-3} s, the ionic level populations achieve equilibrium, that is within the timescale (n_e \tau \simeq 1.0 \times 10^{-5} - 5.0 \times 10^{11} cm^{-3} s) of silicon charge stages to achieve equilibrium at T_e = 1.2 MK that given by Smith & Hughes (2010). Present calculations give a timescale of n_e \tau \simeq 2.0 \times 10^{11} cm^{-3} s for silicon at the same thermal temperature with neutral initial stage (see Figure 5(b)). The ionic fraction shows an excellent agreement with the data of Bryans et al. (2009) when the plasma evolves to equilibrium (see the marked symbols in Figure 5(b)). The electron density is about 10^{10} cm^{-3}, which is a typical value for active regions before the flare event (Brosius et al. 2000). So non-equilibrium effects should be considered when analyzing the spectra of solar flares with high time cadence (<10 s, i.e., SDO).

Effects from metastable populations are also explored on the time evolution of level populations, where two super-levels [L] and [H] will be constructed to take the contribution of the recombination and ionization from/to neighboring ions into account, respectively. A time-dependent ionic fraction is used here. However, an equilibrium assumption has been adopted for neighboring ions when obtaining their level population. The product of metastable level populations and recombinations/ ionizations \sum_i n_i^{q+1} \alpha_i or \sum_i n_i^{q+1} \alpha_i' forms the matrix elements relevant to the two super-levels [L] and/or [H]. The metastable populations are found to be slightly delayed from the time of the level population by ~40–80 ms to achieve equilibrium (see the dashed-dot curves in Figure 5(a)).
3.1.3. Effect from Metastable Level Population

Present available ionization equilibrium data (Mazzotta et al. 1998; Bryans et al. 2009) that is extensively used by the astronomical community are from calculations at the low-density limit (see the top panel in Figure 6). However, many weak density-sensitive emission lines are detected, which are usually populated by excitations from metastable levels; i.e., metastable population should play a role on ionic distribution in equilibrium plasma. Some literatures also attribute observed discrepancies to be a metastable effect. In this work, we investigate this effect on ionic fraction by using the level-resolved ionization and recombination data mentioned in the above section. Here, no line radiation will be considered, the Equations (1)–(6), will be simplified to be

\[
\frac{d}{dt} n_i^{q+} = n_e \left[ \sum_{j=0}^{m^{q+1}} n_j^{(q+1)+} S_{ji}(T_e) + \sum_{j=0}^{m^{q+1}} n_j^{(q+1)+} \alpha_{ji}(T_e) \right] - n_e \left[ \sum_{j=0}^{m^{q+0}} n_j^{q+} S_{ji}(T_e) + \sum_{j=0}^{m^{q+0}} n_j^{q+} \alpha_{ji}(T_e) \right].
\]  

(15)

First, we calculate the ionic fraction of silicon in equilibrium plasma at a low-density limit with the Chianti version 7 database (see the solid curves in the bottom panel in Figure 6), which agrees well with the data of Bryans et al. (2009). That is the present solver for ionic fraction is correct. By using the present ionization data from FAC calculation without contributions from metastable populations (e.g., only the ionization from the ground state is included), present ionic fractions (dashed-dot curves in the bottom panel of Figure 6) slightly shift to higher temperatures. This small difference can be explained by the small differences in collisional ionization data as illustrated in Section 2.

Second, we calculate the ionic fraction of silicon with metastable contributions at an electron density of 10^{10} cm^{-3} (see dashed curves in the bottom panel of Figure 6). Here, we adopt a different approach from the Generalized Collisional-Radiative (GCR) method adopted by the ADAS team (Summers et al. 2006; Loch et al. 2009). There are two separate calculations to be done in the present calculation. First, we obtain the metastable and/or low-excited level population \( n_i^{q+0} \) (hereafter the second upper-script “0” denotes initial ground and metastable populations) of each ion without contribution from ionization and/or recombination at equilibrium. Then the ionization \( S_{ji} \) and recombination \( \alpha_{ji} \) rates of ground and metastable levels in Equation (15) will be multiplied by the initial population \( n_i^{q+0} \) or \( n_i^{q+0} \) for each ion. So we get the \( A \) matrix in Equation (7) with matrix elements of \( S_{ji} n_i^{(q+1)+0} \) and \( \alpha_{ji} n_j^{(q+1)+0} \). The dimension of this matrix depends on numbers of ground and metastable levels of an iso-nuclear series. For example, there are \( m = \{m_1, m_2, m_3, \ldots, m_{15}\} \) where \( m_i \) is the metastable number of \( Si_i \) with a charge of \( q+1 \) of 14+i+1, which is determined by the maximum level index in ionization and recombination data files) metastable levels for various charged silicon ions. We will construct a \( A \) matrix with a \((15+m) \times (15+m)\) dimension.
The resultant values $n_i^{q+}$ in Equation (15) are summed to obtain ionic fraction $\sum_{m=0}^{\infty} n_i^{q+}$ of $q+$ charged ion according to its metastable number $m_i$. Figure 6 demonstrated that the inclusion of metastable populations have an apparent effect on ionic fraction at $n_e = 10^{10} \text{cm}^{-3}$. For some ions, the difference can be up to a factor of two. Moreover the temperatures of peak abundance (i.e., Si viii) shift to lower temperatures by $\sim 8\%$ for some ions.

In comparison to the treatment of the GCR method in the ADAS package, the calculations for line emission and ionization distribution are performed separately in the present sasal method. The first-step procedure in the calculation of ionization distribution mentioned above is equivalent to the second terms of the Equations (6)–(9) in the paper of Loch et al. (2009), where the effective total ionizations or recombination rates of ground/metastable levels include the direct ionizations from ground/metastable levels and effective excitations to other metastable levels followed by ionizations to next higher charged ions (Dickson 1993). Here, the effective excitations are realized by solving level populations without ionization and recombination contributions from neighboring ions. This is the main source of the present approximation than the GCR method. For the line emissions in equilibrium, the present treatment is similar with that for a time-dependent level population discussed in the above subsection. The contribution from level-resolved impact ionization and/or a recombination of metastable levels are also included from the neighboring two ions. In principle, the present model partly ignores the cross-coupling effects in line emissions and ionization distribution. But these effects are expected to be small for most astrophysical and/or laboratory plasmas. A qualitative benchmark is still necessary by a direct comparison with GCR calculation with the same data source in the near future, but that is beyond the scope of the paper.

### 3.2. Photoionized plasma

There are several modeling codes for photoionized plasmas, such as, Cloudy maintained by Ferland et al. (1998) or Xstar (Kallman & Bautista 2001), as well as PhiCRE constructed by Wang et al. (2011) for laser irradiated plasmas. For completeness, we also complement the spectroscopic module for photoionized plasma in the present sasal package, which adopts the data as mentioned in Section 2 and gives a brief test below for the present model. At present, only the blackbody radiation field is setup and used in this work, while other radiation fields are routinely in plan and easily setup by idl keywords. As stated in Section 2, the optically thin assumption was adopted in the present model, then no radiative transfer is treated in this work. Moreover, an external constant blackbody radiation field is assumed to investigate the charge state distribution.

In calculation of charge stage distribution of PI plasma, only total PI and dielectronic/radiative recombination are included, Equations (1)–(6) are simplified to be

$$
\frac{d}{dt} n_i^{q+} = n_e [n_i^{q+} (q+1)^+ - \alpha^{q+} (T_e)] + \gamma [n_i^{q-1+} (q-1)^+ (E) - n_i^{q+} \phi^{q+} (E)],
$$

where $\theta$ and $\alpha$ denote the total PI and recombination rate coefficients, respectively. Figure 7 (bottom panel) shows the ionic fraction in photoionized plasma over temperature ($T_e$) $0$–$28 \text{eV}$ of the blackbody radiation field. For comparison with collisional plasma, the ionic fraction in collisional equilibrium is plotted in top panel. For helium-like silicon (Si xiii), it has a peak abundance around $T_e = 400 \text{eV}$ in collisional plasma, but it can achieve peak abundance at the radiation field of $T_e = 25 \text{eV}$. We further use the sasal model to analyze the charge state distribution of a photoionized iron plasma performed by Foord et al. (2004) at the Sandia National Laboratory Z-pinch facility. The present result shows a good agreement with the experimental value at the plasma temperature of $100 \text{eV}$, as well as with previous predictions$^9$ from the well-known GALAXY, CLOUDY codes at $T_e = 150 \text{eV}$ and recent PhiCRE model at $T_e = 92 \text{eV}$ (Wang et al. 2011) (see Figure 8). In the present prediction, an experimentally measured electron density of $2.0 \times 10^{19} \text{cm}^{-3}$ is adopted.

The time evolution of ionic fraction is also explored for silicon in photoionized plasma (see Figure 9), where the electron density is $10^{14} \text{cm}^{-3}$ and the radiation temperature

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$^9$ There are small uncertainties inherent to those data points because they are sampled from a published paper.
is 30 eV. This demonstrates that the maximum timescale \((n_e t)\) is \(\sim 2.0 \times 10^{11} \text{ cm}^{-3} \text{ s}\) to achieve equilibrium at \(T_e = 30 \text{ eV}\). For high-energy density plasma \((n_e = 10^{20} \text{ cm}^{-3})\) in the laboratory, the maximum timescale to achieve equilibrium is \(\approx 6.0 \times 10^{11} \text{ cm}^{-3} \text{ s}\) at \(T_e = 30 \text{ eV}\). This timescale also depends on radiation temperature.

Discrete emissions excited by recombination are important spectroscopic evidence in a tenuous X-ray photoionized medium (Paerels et al. 2000), presumably the stellar wind from the Wolf–Rayet companion star (van Kerkwijk et al. 1992). Cyg X-3 shows a bright, purely PI-driven spectrum and may provide a template for the study of the spectra of more complex accretion-driven sources, such as active galactic nuclei. By using the present SASAT model, we analyze the discrete recombination emissions of highly charged carbon by using level-resolved PI cross sections that are available from Nahar’s Web site. By using Milne relation, we get the radiative and dielectronic recombination rates. Figure 10 shows the spectra of He-like carbon in photoionized plasma radiated by a blackbody source with \(T_R = 40 \text{ eV}\). For comparison, its spectra in coronal-like plasma with \(T_e = 100 \text{ eV}\) are also overlapping. This clearly demonstrates that the recombination process favors the population of the metastable level \((1s2e^2S_1)\) of the forbidden transition \((f\text{ line})\), that differs completely from the case of collisional plasma, where resonance transition \((1s2p^2P_{1/2} \rightarrow 1s^21S_0, r\text{ line})\) is the strongest one. Such characteristics are usually used to diagnose the heating mechanism of the emitting region in astrophysical objects. Using the level-resolved dielectronic and radiative recombination rates compiled in Section 2, we further analyze the ratio of \(f(r + i + j)/(i, j \text{ lines})\) for \(\text{Si}^{\text{xii}}, \text{S}^{\text{xv}}\) and \(\text{Ar}^{\text{xvi}}\) in Chandra observation for Cygnus X-3 (Paerels et al. 2000). The resultant ratios are 1.51 (\(\text{Si}^{\text{xii}}\)), 1.32 (\(\text{S}^{\text{xv}}\)), and 0.97 (\(\text{Ar}^{\text{xvi}}\)) that are consistent with Cygnus X-3 observations of 1.3, 1.0, and 0.8, respectively, where we adopt a temperature of 50 eV estimated by Paerels et al. (2000) according to the shapes of \(\text{Si}^{\text{xiv}}\) and \(\text{S}^{\text{xv}}\) RRC features. The estimated temperature \((\sim 60 \text{ eV})\) based on the present RRC emissivity is roughly consistent with the estimation of Paerels et al. (2000) from an inspection of Figure 2 in their work (see the bottom panel of Figure 10).

For completeness, the spectrum due to the CX process is also overlapping in Figure 10, where the projectile \((\text{C}^{\text{vi}})\) velocity is 200 \(\text{km s}^{-1}\). Its resultant spectrum is similar with that in photoionized plasma. The forbidden transition line is the strongest one. This kind of line formation will be discussed in a below subsection.

### 3.3. Geocoronal Plasma

One of the best studied comets is Chandra C/1999 S4 (LINEAR) observation (Lisse et al. 2001), because of its good signal-to-noise ratio \((S/N)\). To discuss our spectral model, we compared our findings with earlier studies of this comet. Although earlier charge-exchange (CxEE) models (Wegmann et al. 1997; Cravens 1997; Häberli et al. 1997) can explain the observed X-ray luminosity well, their spectral line shape predictions do not agree with the observation of the three line ratios of 2.3:4.5:1 at 400, 560, and 670 eV. Beiersdorfer et al. (2003) interpreted the C/1999 X-ray spectrum by fitting it with their EBIT spectra. That model takes multiple electron capture into account implicitly, but the collision energies of 200 eV to 300 eV \((\sim 30 \text{ km s}^{-1})\) are far away from the velocities \((\sim 300–800 \text{ km s}^{-1})\) of solar winds. (Bodewits et al. 2007; see Figure 3) demonstrated that the hardness ratio has a strong dependence on the collision velocities below 300 km s\(^{-1}\), implying an overestimation for higher-order transition lines than \(n = 2 \rightarrow 1\) transition in the work of Beiersdorfer et al. (2003). However, unexpected high C v fluxes or low C vi/C v ratios were predicted by Bodewits et al. (2007). A small contribution from other ions in the 250–300 eV are pointed out by them, which was not included in their model. Otranto et al. (2007) included contributions from the Mg ix, Mg x, and Si ix ions by using the CTMC intensities of the Balmer transitions corresponding to a bare projectile with charge equal to that of the projectile.
The available data set for LINEAR 1999 S4 in the Chandra public data archive are listed in Table 2 before its breakup. The data reduction is performed by using the Chandra Interactive Analysis of Observations (CIAO) software (ver. 4.5)\(^\text{10}\) and by following the science threads for imaging spectroscopy of solar system objects. In the data reduction, the source region covers the S3 chip with a circle region with a radius of 4.56, while the background is extracted from S1 chip with a circle region (radius of 3.78). The data set with Obs_ID of 1748 was not included in the our analysis due to its low S/N. The other seven spectra were combined by using the combine spectra tool to get a high S/N spectra. Correspondingly, associate auxiliary response files and energy dependent sensitivity matrices were obtained by this tool simultaneously. The resultant observational spectra is presented by symbols with error bars in Figure 11. We also notice the difference of the comet LINEAR observations between the present extraction and Lisse et al. (2001)'s data before its breakup as well as the data adopted by Otranto et al. (2007). This is due to different source regions adopted in the spectral extraction as illustrated by Torney (2007). In the work of Lisse et al. (2001), they adopted EUVE spatial profiles for the full extent of the comet to correct the Chandra X-ray flux because the comet overfills the S3 chip and falls outside its field of view. However, the relative emission line fluxes have small differences between the present observation and previous ones and are within uncertainties. This means the comparison of relative solar wind abundance with published values that will be discussed in the following subsection, is still feasible.

### Table 2

| Obs_ID | Exposure Times (ks) | Average Count Rate | Event Count | Start Time |
|--------|---------------------|--------------------|-------------|------------|
| 584    | 0.95                | 3.00               | 2839        | 04:29:19   |
| 1748   | 1.18                | 2.83               | 3331        | 05:06:19   |
| 1749   | 1.18                | 2.98               | 3501        | 05:31:29   |
| 1750   | 1.19                | 2.85               | 3384        | 05:56:39   |
| 1751   | 1.18                | 7.13               | 8383        | 06:21:49   |
| 1752   | 1.19                | 6.81               | 8093        | 06:46:59   |
| 1753   | 1.18                | 7.46               | 8812        | 07:12:09   |
| 1754   | 1.36                | 4.06               | 5516        | 07:37:19   |

3.3.1. Observation Data for LINEAR

The fitting procedure is done in the sherpa package of CIAO version 4.5\(^\text{10}\). A multi-Gaussian model is constructed based on the spectral lines calculated by our SASAL package, as the following formula,

\[
I_{\text{theo}}(\gamma) = \sum_i A_i \sum_j G_{ij}(\gamma, E_{ij}) \epsilon_{ij},
\]

where \(A_i\) is ionic fraction, \(G_{ij}(\gamma, E_{ij})\) is Gaussian profile of a given transition \(i \rightarrow j\) with the transition energy of \(E_{ij}\) and a given line width, and \(\epsilon_{ij}\) is CX line emissivity.

In Figure 11, we present our CXE fit X-ray spectra for Linear C/1999 S4 with thousands of lines at velocities of 300 km s\(^{-1}\) (a, fast solar wind) and 600 km s\(^{-1}\) (b, slow solar wind), respectively. The collision velocity of 600 km s\(^{-1}\) adopted here is consistent with the ACE-SWEPAM and SOHO-CELIAS online data archive (592 km s\(^{-1}\)). The line width is set to be 50 eV, being consistent with that adopted by Bodewits et al. (2007) and Lisse et al. (2001). It is narrower than the intrinsic line-width of 110 eV FWHM of the ACIS-S back-illuminated CCD (Garmire et al. 2003).\(^\text{11}\) As stated by Lisse et al. (2001), it is not significant statistically. In this model, we include contributions from Mg x, Si x, and Ca xiv CX emissions. But no Ca x\(^{14+}\) species can be estimated in both solar winds. The inclusion of Mg x and Si x CXE emissions improves the fitting to the spectra between 200 eV and 300 eV with reduced \(\chi^2 = 1.46\), that region was omitted in the analysis of Bodewits et al. (2007). The resultant ionic abundances in solar winds by this fitting are presented in Table 3. For the O x\(^{8+}\), C x\(^{6+}\), and N x\(^{6+}\) ions, the present results are consistent with previous estimations based upon models. Since there is significant contamination from C v and Mg x emissions below 300 eV, no C x\(^{5+}\) fraction is predicted in the fast (600 km s\(^{-1}\)) solar wind. However, a high fraction for Mg x\(^{10+}\) is predicted in the solar wind. Moreover, the predicted Si x\(^{10+}\)

\(^{10}\) http://cxc.cfa.harvard.edu/ciao/

\(^{11}\) http://cxc.harvard.edu/proposer/POG/html/ACIS.html
species (0.10) is consistent to its fraction (0.12) listed by Schwadron & Cravens (2000) for the slow wind in their Table I, being significantly lower than that listed for the fast wind by them. Contributions from unresolved emission lines of Mg x and Si x were not included by Bodewits et al. (2007) and Otranto et al. (2007). And only 10 emissions were included by Krasnopolsky (2006) without contribution from N6+.

In the fitting with the CXE spectra at the collision velocity of 300 km s\(^{-1}\), no Si\(^{10+}\) and Ca\(^{14+}\) ions are derived, and the reduced \(\chi^2 = 1.79\) becomes larger. This indirectly confirms that the collision energies between recipients and atom/molecular donors play important roles on spectroscopic analysis for geocoronal plasmas. Correspondingly, we can estimate the origins of solar wind ions on the solar surface that arrive with comets or the planet atmosphere as demonstrated by Bodewits et al. (2007).

In summary, the complement of MCLZ method makes the spectroscopic analysis of CX plasmas feasible for the astronomical community, and it confirms that it is reliable. The reliability of hydrogen models are also appropriate, which is presented by Smith et al. (2012).

4. SUMMARY AND CONCLUSIONS

In this work, we presented a spectroscopic model for various astrophysical and/or laboratory plasmas, including coronal-like, photoionized, and geocoronal plasmas under the optically thin assumption.

1. For coronal-like plasmas, we construct two different modules for thermal and non-thermal (e.g., EBIT) electrons. Here the original collision strengths are compiled into the database, and offline calculation can be done for the \(R\)-matrix excitation data on the local server. This procedure will avoid the invalidity problem of detailed balance of effective collision strength between excitations and de-excitations for non-thermal electrons that extensively adopted by spectroscopic community. So any form of electron energy distribution can be incorporated into this module. In modeled monoenergetic case (EBIT), some emissions are strengthen, while others are weaken than those in thermal plasma.

2. Effect of metastable population on charge stage distribution and level population are explored by using level-resolved ionization and recombination data. It is found to be small at low-density plasma.

3. Time evolutions of ground and metastable level population are explored and are found to achieve equilibrium at \(n_{e1} \sim 1.5 \times 10^9\) cm\(^{-3}\). This value is comparable to the timescale \((n_{e1} \lesssim 2.0 \times 10^{14}\) cm\(^{-3}\) s\(^{-1}\)) of charge stages for achieving equilibrium. So when plasma departures from the equilibrium status, it means that not only the ionic states deviate from equilibrium, but also the level populations possibly depart from equilibrium at low-density plasma.

4. A module for photoionized plasma with a blackbody radiation field is complemented in this model for charge stage distribution and line emissions based upon a fitted total cross section and a partial level-resolved cross section. Although the present model is not a self-consistent solution to most astrophysical photoionized medium, we use it to successfully analyze the discrete recombination emissions and RRC features in the photoionized wind of Cyg X-3, as well as the charge state distribution of a laboratory plasma.

5. The CX spectroscopy of comet–LINEAR is investigated again here by using the online parameterized MCLZRC cross-section calculation under the present sasal database. This makes the spectral fitting and analysis feasible for various solar wind ions besides bared, H-like, and He-like ions. The application to comet–LINEAR reveals that the present resultant ionic fraction shows a good agreement with previous ones for O\(^{6+}\), C\(^{6+}\), N\(^{6+}\), and Mg\(^{10+}\) ions, wherever a low and high ionic fraction derived for C\(^{5+}\) and N\(^{7+}\) than previous ones, respectively. This is due to inclusion of other emissions and low-resolution of the LINEAR spectra. High-resolution spectroscopy will clarify this discrepancy. Moreover, the velocities of solar wind ions have a significant effect on the determination of ionic fractions. Additionally, some available \(l\)- and/or level-distributed cross section are compiled into the present sasal database.

In conclusion, we set up a self-consistent spectroscopic modeling package–sasal for coronal-like, photoionized and geocoronal plasmas at equilibrium and non-equilibrium. It is not only a combination of previous available modeling codes, but also an extension on metastable effect, time evolution and CX dominant plasma, etc. Although some assumptions were made, test applications prove the sasal model to be reliable for many astrophysical and laboratory plasmas. The spectroscopic model for astrophysical and laboratory cases benefits the community of laboratory astrophysics due to their inherent differences between them.
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