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X-ray spectral diagnostics for satellite lines of H-like Mg ions measured by a high resolution spectrometer

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Abstract

X-ray spectra of H-like Mg ions produced in a laser plasma have been measured by space-resolved high-resolution spectroscopy. We identified satellite lines near Lyα lines, 2lnl′ − 1snl′ + hv for n = 2, 3, and 4. We construct a collisional-radiative model including the doubly excited states for the intensity ratios of satellite lines. We use atomic data calculated by different methods for satellite lines and compare the results. We derive the electron temperature and density of the laser-produced plasma by a new technique using intensity ratios of only satellite lines. This technique is useful because the Lyα lines are often affected by opacity.

Keywords: H-like Mg ions; Plasma diagnostics; Satellite line; X-ray spectra

1. INTRODUCTION

In high temperature and high density plasmas, satellite lines emitted through doubly excited states are important for plasma diagnostics. Satellite lines have been widely used for plasma diagnostics of solar flares (e.g., Dubau & Volonte, 1980; Bely-Dubau et al., 1982), Tokamak plasmas (e.g., Bitter et al., 1984; Kato et al., 1987), and laser-produced plasmas (Fujimoto et al., 1981; Demir et al., 1997), especially for dielectronic satellite lines of Li-like ions. In this article we study the satellite lines of He-like ions in detail. We have made a collisional-radiative model (CRM) for H-like and He-like ions including the doubly excited states. X-ray spectra of H-like Mg ions were measured from a laser-produced plasma with a high-resolution spectrometer by Rosmej et al. (1999, 2001). We identify satellite lines for 1snl lines (n = 2–4) and analyzed the spectra using our CRM. We compare three kinds of atomic data for spectral analysis. We derived temperatures of 180, 200, and 210 eV at three points imaged by the spectrometer. The derived electron density is 5 × 10^{20} cm^{-3}.

2. EXPERIMENTAL SETUP

X-ray line spectra with high spectral resolution (λ/Δλ ~ 5000) were measured at the helix-laser facility at GSI-Darmstadt (Rosmej et al., 1999, 2001). The laser is a 100-J Nd-glass laser (λ = 1.046 µm), with a pulse width of 15 ns and energy of 17 J. A massive Mg target is irradiated at normal incidence. The focal spot diameter on the target is 500 µm. X rays generated at the target are observed with a spherically bent mica crystal in second-order refraction providing simultaneous high spatial and spectral resolution. The mica crystal was used in order to have a spherical geometry for the Bragg crystal, which permit simultaneous high spectral and spatial resolution while maintaining high luminosity (because no slit is required for the space resolution). The second order was used to increase the resolution. In first order, the imaging properties of the spherical geometry are not so good because the Bragg angle is too small. The spatial resolution in the z-direction is 14 µm. Because X-ray film is used to record the spectra, there is no time resolution.

We have analyzed spectra from three different positions: “center,” “+170 µm” and “−170 µm.” The “center” position corresponds to the crossing points of the laser beam and the surface of the target. The “+170 µm” position corresponds to a position separated 170 µm from center in the normal direction. The “−170 µm” position corresponds to a
position below the center point. The observed spectra are shown in Figure 1.

3. COLLISIONAL-RADIATIVE MODEL FOR SATELLITE LINES

Normally collisional-radiative models (CRM) include only singly excited states, and the doubly excited states, which lie under a singly excited state, are not explicitly included. However we observe many satellite lines that are emitted through the doubly excited states in X-ray spectra from laser-produced plasmas, solar flares, and magnetic confined plasmas such as tokamak. We have constructed a CRM of the H-like and He-like system including the He-like doubly excited states including the n = 2 (2s and 2p) levels for H-like ions and the levels up to n = 3 (3s, 3p, and 3d) for H-like levels. Details of this model are given in Yamamoto et al. (2002) and Kato et al. (2001).

3.1. Energy level

In our CRM the ground state 1s$^2$ and singly excited states 1snl, doubly excited states 2l$'$nl and 3l$'$nl for He-like ions, and 1s, 2l, and 3l states for H-like ions are included. The total number of levels is 367: 1snl (60 states), 2l$'$nl (230 states), and 3l$'$nl (70 states). For singly excited states, 1snl, n = 2 states are resolved in fine structure levels; for the states with 3 ≤ n ≤ 7, the different total angular moment J states are combined keeping L and S separate; for the levels with 8 ≤ n ≤ 10, the total orbital angular momenta L are combined but spin S are kept separate; and for the levels with 11 ≤ n ≤ 20, they are averaged into the principal quantum number n. For doubly excited states, 2l$'$nl, with 2 ≤ n ≤ 5 are resolved into fine structure levels, and the levels with 6 ≤ n ≤ 20 are combined into the averaged excited states as 1snl states. For doubly excited states, 3l$'$nl, n = 3 levels are averaged with total angular moment J, and 4 ≤ n ≤ 20 are averaged with orbital quantum number l. In Figure 2 the schematic energy level diagram for our CRM is shown.

3.2. Rate equation

An emission line intensity is calculated using a population density of an upper level multiplied by a radiative transition rate. Population densities are calculated by rate equations as follows:

$$\frac{dN_i}{dt} = -\sum_j W_{ij}N_j + \sum_j W_{ji}N_j,$$

where $W_{ji}$ is a total transition rate from j state to i state.

Atomic processes considered in our model are electron impact excitation/de-excitation, ionization/three-body recombination, radiative recombination, and dielectronic capture, radiative transition, and autoionization. Collisional atomic data (excitation and ionization) for singly excited states 1snl and for doubly excited states 2l$'$nl are the same as used in Yamamoto et al. (2002). Collisional excitation rate coefficients between doubly excited states 2l$'$l$'$ are taken from Goett et al. (1983) and from 1s2l to 2l$'$l$'$ are taken from Sampson et al. (1983). The transition rates between doubly excited states 3l$'$nl are calculated using the HULLAC code (Bar-Shalom et al., 1988).

Eq. (1) is solved assuming quasi-steady state for doubly and singly excited states. Under this assumption we can write the steady-state population densities $N_i$ of excited states as a linear combination of the population densities of 1s$^2$, 1s, 2s, 2p, 3s, 3p, and 3d as follows:

Fig. 1. a: The measured spectrum near H-like Mg Ly$α$ lines. The spectrum is obtained from “center.” b: The measured spectrum near Ly$α$ lines with identification for satellite lines.
$N_i = \sum_y r_i^y N_e N_y,$  \hspace{1cm} (2)

where $r_i^y$ and $N_e$ are the population density coefficient and the electron density, respectively. The suffix $y$ indicates the ground states of He-like ions $1s^2$ and H-like ions $1s$, and H-like excited states, $2s, 2p, 3s, 3p,$ and $3d$.

Line intensities are then obtained by multiplying the population density $N_i$, and radiative transition rate $A'$ as follows:

\[ I_s = N_i A'. \]  \hspace{1cm} (3)

### 3.3. Discussion of the averaged level model for satellite line spectra

When we have to take into account many excited states in CRM, we can consider the averaged levels for simplicity. In an averaged level model, the population densities of detailed levels are obtained distributing the averaged level population density according to the statistical weights. Then the line intensities for detailed levels are calculated from the population densities in averaged model. We find the difference in satellite line intensities between an averaged model (the level with different $J$ but with the same configuration is combined to one level) and an individual level model (the levels are separated with $J$) separated with fine structure levels. Comparison with an averaged model described in Yamamoto et al. (2002) and Kato et al. (2001) and an individual model calculated in this article is discussed in this section. Both models use atomic data from the MZ code (Vainshtein & Safronova, 1978, pers. comm., 2000). Comparisons for satellite line spectra by two different models are shown in Figure 3 for (a) $1s3l-213l'$, (b) $1s3l-214l'$ and (c) $1s3l-215l'$. To avoid the density effect on line intensities, electron density in the calculation is assumed to be $1 \text{ cm}^{-3}$, which corresponds to the low-density limit.

The averaged model assumes the population densities are proportional to the statistical weights of the levels. There-

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**Fig. 2.** The schematic energy level diagram for our CRM.

**Fig. 3.** Comparison of satellite line spectra between models with averaged levels (solid line) and individual levels (dotted lines). Electron and ion temperatures are assumed to be 200 eV and 180 eV, respectively. Electron density $N_e$ is assumed to be $1 \text{ cm}^{-3}$, and the instrumental width is taken to be 1.5 mA. a: $1s3l-213l'$; b: $1s4l-214l'$; and c: $1s5l-215l'$ transitions.
fore, generally, the intensities by an averaged model give larger intensities than the individual model in total. We can say that the intensities in an averaged model correspond to those in a high density limit where the collisional processes are dominant.

Comparison between averaged and individual models for 1s3l–2l′3l′ transitions are shown in Figure 3a. Between 8.38 Å and 8.50 Å, satellite line intensities by the averaged model are larger than those by the individual model except line f (1s3d 1D2–2p3d 1F3, 8.406 Å). In the averaged model three 2p3d singlet levels (1P, 1D, and 1F) are combined into one 2p3d singlet level. Because the autoionization rate for 2p3d 1F3 is larger than those of other 2p3d 1P, 1D levels, the population density of 2p3d 1F becomes smaller in the averaged model compared to an individual model. When the electron temperature is derived from the intensity ratio \( I_i/I_j \), the predicted temperature might be overestimated in an averaged model compared to an individual model. When the autoionization rate for 2p3d 1P, 1D levels is small, the population density in an individual model is larger by a factor of 10–10³ than from the averaged model because the effect of other 2p3d levels becomes large due to the effect of other 2p3d levels where the dielectronic capture rates are large. However in the averaged model the population density becomes large due to the effect of other 2p3d levels where the dielectronic capture rates are large. For 1s4l–2l′4l transitions, in the wavelength range longer than 8.43 Å, the agreement between the two models is good. However, the spectra from the averaged model in the range 8.41–8.43 Å is larger than that from the individual model by a factor of 2–3 as shown in Figure 3b. The line intensities between 8.4157–8.4158 Å are stronger from the individual model than from the averaged model because the autoionization rates from 2p4f 3D, the upper levels for these transitions, are large compared to other 2p4f triplet levels.

4. ATOMIC DATA

To interpret the observed spectra, atomic data are very important. We compare here three different theoretical data sets calculated using (1) MZ code by Vainshtein and Safronova (1978) and U.I. Safronova (pers. comm.), Vinogradov et al. (1975), (2) a code based on relativistic many-body perturbation theory combined with complex rotation by Lindroth (1975), and (3) a code based on relativistic many-body perturbation theory by Safronova (MBS; pers. comm.).

We compare the atomic data for satellite lines 1s2l–2l′2l, 1s3l–2l′3l, 1s4l–2l′4l, and 1s5l–2l′5l. Three atomic data sets by MZ, MBS, and MBL are compared for the wavelengths, radiative transitions, autoionization rates, and intensity factor \( Q_a \):

\[
Q_a = \frac{g_i A_i^{A_i}}{\sum A_i + \sum A_i^{A_i}}
\]

where \( g_i \) is a statistical weight for upper state \( i \), \( A_i \) is the radiative transition rate from level \( i \) to \( j \), and \( A_i^{A_i} \) is the autoionization rate from level \( i \). The data by MZ are represented by the LS coupling scheme and those by MBS and MBL are \( jj \) coupling. Generally for 2l′2l and 2l′3l lines, agreements are good. Large differences are found for 2l′4l and 2l′5l lines between MZ and many body theory (MZ and MBL). In the following, the differences in atomic data are represented by percentages relative to the values given by the MZ method (e.g., \( (MBS - MZ)/M \times 100 \)).

Comparison of the different atomic data, MZ, MBS, and MBL, is given in Figure 4 for \( n = 2 \), \( n = 3 \), \( n = 4 \), and \( n = 5 \) transitions in a form of convoluted intensity factor, \( Q_a \times P(\lambda) \), where \( P(\lambda) \) is a line profile of Voigt type.

Most of the data for 1s2l–2l′2l transitions, the \( A_i \) and \( A_i^{A_i} \) values agree within ±20%. The difference in intensity factor \( Q_a \) for these transitions is about 10%. The largest difference for \( A_i \) values is 30% for the 2p2 3P state, which is the upper state of line d. The disagreement in \( Q_a \) for d line is also 30% for both MBS and MBL data. For J line (1s2p 1P–2p2 1D2), which has the largest \( A_i \) in satellite lines, wavelength of MBS is 1.6 mÅ shorter than MZ and MBL.

The difference for 1s3l–2l′3l transitions are larger than those for 1s2l–2l′2l transitions. The differences of \( A_i \) for 2p3d 1F3, the upper level of line f, are 40% for MBS and 5% for MBL, and the differences of \( Q_a \) are 13% for MBS and 7% for MBL, respectively. The strongest line in this wavelength range is 1s3d 3D1,2,3–2p3d 3F2 and the atomic data for this transition agree well.

The discrepancies for 1s4l–2l′4l transitions are much larger than those for \( n = 2 \) and 3. Especially, \( A_i \) values by MZ for 2p4f 3D1,2,3, which are the upper states of satellite lines in the wavelength range of 8.4157–8.4158 Å are larger by 1–4 orders of magnitude than those by MBS and MBL. Therefore, \( Q_a \) values of these transitions by MZ are also larger by a factor of 10–10³ than MBS and MBL.

For \( n = 5 \) transitions, \( Q_a \) values of transitions from the upper states 2s5f 3F and 2p5f 3D by MBL are smaller by a factor of 10–10³ than those by MZ, because the autoionization rates by MBL are smaller than MZ by a factor of 10³–10⁴. Therefore the large difference is found at around 8.417 Å as shown in Figure 4d. The \( Q_a \) value for 1s5d 3D1–2p5d 3F4 (8.426 Å) transition by MBL is 20% of that by MZ because the autoionization rate is about 20% and the radiative transition rate is 30% of those by MZ.

5. PLASMA DIAGNOSTICS FOR \( T_e \) AND \( N_e \) USING SATELLITE LINE INTENSITY RATIOS

Because the satellite line intensities depend on electron temperature \( T_e \) and density \( N_e \), the satellite line intensity ratios depend on \( T_e \) and \( N_e \). The intensities in this section are calculated for an ionizing plasma where the doubly excited states are populated by dielectronic capture from the 1s state only.

The density dependence is mainly caused by the collisional process through \( l \)-changing with the same quantum number \( n \). Electron density dependence for several line
Figure 5. Because the dielectronic capture rate to low densities. With increasing electron density, population density of states is larger than that of 2p\(^2\) 3P\(_2\) at higher densities than 10\(^20\) cm\(^{-3}\). The intensity ratios of satellite lines at 200 eV in an ionizing plasma. Thin lines are intensity ratios by MZ for \(I_a/I_j\) (solid line), \(I_s/I_j\) (dotted line), and \(I_I/I_j\) (dot-dashed line). Bold dot-dashed line is for \(I_d/I_j\) by MTL.

Electron temperature dependence of several line intensity ratios at \(N_e = 10^{20}\) cm\(^{-3}\) are shown in Figure 6. The ratio \(I_d/I_j\) strongly decreases with increase of temperature. The intensity ratios of the satellite lines to the resonance line have been often used to estimate electron temperature in high temperature plasmas (e.g., Kaot et al., 1998). However in our case we do not use this ratio because Ly\(\alpha\) might be affected by opacity as mentioned in Section 2. The intensity ratios of lines, which have the same quantum number as an upper state, have no temperature dependence. The line intensity \(I_d/I_j\) can be used for electron density diagnostics in the electron density range \(N_e \approx 10^{20}\) cm\(^{-3}\). Electron density derived from \(I_d/I_j\) by MBL gives larger values than that by MZ.
temperature and density for the ratio \( I_c/I_l \) can be used to define a reference line ratio in the measured spectra.

6. SPECTRAL ANALYSIS

We analysed three kind of spectra measured from center, \(-170 \, \mu\text{m}, \) and \(+170 \, \mu\text{m} \). The intensity ratio \( I_f/I_l \) has a strong temperature dependence and \( I_d/I_l \) has density dependence as shown in Section 5. We used mainly these two intensity ratios to derive the electron temperature and density. Among three sets of atomic data compared in Section 4, we used MZ and MBL data for our spectral analysis and compared the derived plasma parameters. The satellite line intensities are calculated by our collisional radiative model including the dielectronic states. Ionization equilibrium is assumed in our analysis.

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Theoretical spectra using the atomic data by MZ and MBL are shown by dotted lines in Figure 7a, b, respectively. In the MZ case, the electron density $N_e$ is obtained approximately $5 \times 10^{20} \text{ cm}^{-3}$ from the intensity ratio of $I_d/I_l$. The temperature $T_e = 200 \text{ eV}$ is derived from the intensity ratio $I_c/I_l$ with MZ atomic data. This temperature corresponds to the high temperature limit to fit the spectra in the wavelength range near the foot of Lyman $\alpha$. When we use the atomic data by MBL, the derived temperature $T_e = 230 \text{ eV}$, which is higher than that by MZ because of the difference of atomic data for the $f$ line. Two broad peaks near 8.43–8.44 Å and 8.44–8.46 Å are consistent with a large number of weak satellite lines, not only from 2$\ell$1 but also 2$\ell$4' and 2$\ell$5'. They are in good agreement with the measured spectra in the case of MZ. On the shorter wavelength side of Lyman $\alpha$ ($\sim$8.415 Å) the calculated spectrum exceeds the measured spectrum as seen in Figure 7a. This excess comes mainly from 1s4f–2p4f lines, which are much stronger by MZ than MBL, as discussed in Section 4. Theoretical spectral feature near Lyman $\alpha$ foot with MBL atomic data agrees with the measured spectra better than that by MZ. Although the satellite lines in 8.44–8.46 Å are in good agreement, the theoretical spectra in 8.43–8.44 Å is too small in the case of MBL. The line intensity ratio $I_c/I_l$ does not depend on temperature and density and should be constant for any condition, as shown in Figures 5 and 6. This intensity ratio can be used to determine the background level. We derived the background level considering the intensity ratio of $I_c/I_l$. However as seen in Figure 7, the theoretical intensity of line $c$ is always smaller than the observed intensity. The atomic data for $c$ might be wrong or there is some dynamic effects in plasma. The ion temperature is assumed to be $T_e = 200 \text{ eV}$ for the theoretical spectra. This value is derived from the observed line profile of $J$ and $c$.

For the spectra of $-170 \mu \text{m}$, we obtained $T_e = 180 \text{ eV}$ and $N_e = 4 \times 10^{20} \text{ cm}^{-3}$ by MZ data. For the spectra of $+170 \mu \text{m}$, we derived $T_e = 210 \text{ eV}$ and $N_e = 5 \times 10^{20} \text{ cm}^{-3}$ as a best fit with atomic data by MZ.

7. SUMMARY AND DISCUSSION

We have constructed CRM including doubly excited states and analyzed X-ray spectra of H-like Mg ions measured at GSI. We identified satellite lines for 2$\ell$21', 2$\ell$31' and 2$\ell$41' transitions from the measured spectra.

We study the density and temperature dependences of satellite line intensity ratios. We proposed the new method for plasma diagnostics using only satellite line intensity ratios. We compared three kinds of atomic data, MZ, MBL, and MBS for spectral analysis. We found a better spectral fit with MZ data than MBT in 8.43–8.44 Å (2$\ell$4' lines). However MBT is better than MZ near 8.415 Å (2$\ell$5' lines).

The plasma parameters are derived with the satellite line intensity ratios. The derived parameters are $T_e = 200 \pm 10 \text{ eV}$ and $N_e = 5 \pm 2 \times 10^{20} \text{ cm}^{-3}$ for the center position, $T_e = 210 \text{ eV}$ and $N_e = 5 \times 10^{20} \text{ cm}^{-3}$ for $+170 \mu \text{m}$, and $T_e = 180 \text{ eV}$ and $N_e = 4 \times 10^{20} \text{ cm}^{-3}$ for $-170 \mu \text{m}$.

We are going to analyze the spectra including the intensity of Ly$\alpha$ lines with the effect of opacity using Monte Carlo simulation. We would like also to study the dynamic effect on the observed spectra.

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