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Detailed Analysis of Spectra from Ga-like Ions of Heavy Elements Observed in High-Temperature Plasmas

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Abstract: This study has systematically investigated the atomic number (Z) dependence of spectra from gallium-like (Ga-like) ions of heavy elements. We have mainly analyzed the experimental spectra recorded in high-temperature plasmas produced in the Large Helical Device (LHD) for various elements with atomic numbers from 57 onward. The measured wavelengths are compared with theoretical values calculated with a multi-configuration Dirac Fock code. As a result, we have successfully obtained Z-dependent wavelengths of several prominent transitions of Ga-like ions, including a magnetic dipole (M1) transition. Many of them have been experimentally identified for the first time in this study. The present results manifest the significant effects of configuration interaction and spin–orbit interaction for highly charged heavy ions.

Keywords: Ga-like ions; heavy elements; soft X-ray spectra; configuration interaction; spin–orbit splitting

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1. Introduction

Extreme ultraviolet (EUV) and soft X-ray emission spectra from highly charged heavy ions are of great interest in a variety of research fields such as nuclear fusion [1,2], industrial light source applications [3,4], and basic atomic physics [5,6]. Among a wide range of ion stages of highly charged heavy ions, gallium-like (Ga-like) ions have a relatively simple ground state configuration, $[Ar]3d^{10}4s^24p$, which includes only three N-shell electrons outside the closed M-shell. Therefore, the energy level structure of Ga-like ions is quite sparse, which leads to a relatively simple emission spectra composed of a few strong isolated lines. The ionization energies of Ga-like ions of the elements with Z = 57–74 are roughly 0.9–2.2 keV. Therefore, high-temperature plasmas or electron beam ion traps (EBITs) with high beam energies are indispensable for experimental studies on Ga-like heavy ions. In fact, the experimental survey for the spectral lines of Ga-like heavy ions has mainly been carried out so far in Texas Experimental Tokamak (TEXT) [7,8] and an EBIT facility at the National Institute of Standards and Technology (NIST) [9–14]. However, experimental investigations of spectral lines of Ga-like heavy ions are still incomplete, and their atomic number (Z) dependencies have not been fully analyzed yet. Regarding the elements with Z = 57–74, for example, EBIT data have been reported only for the elements with Z of 73 and even numbers in 60–74 [9–15], while no EBIT data are available for the other elements.

Magnetically confined torus plasmas are considered to be appropriate for producing spectroscopic data on highly charged heavy ions because of their favorable plasma parameters and the availability of reliable diagnostic tools. From this point of view, we have so far systematically recorded EUV and soft X-ray spectra of highly charged heavy ions in high-temperature plasmas produced in the Large Helical Device (LHD), a magnetically confined torus plasma device at the National Institute for Fusion Science (NIFS) [16–23]. In order to complete the missing experimental data, this article focuses on the Z-dependent properties of the isolated spectral lines of Ga-like heavy ions observed in LHD plasmas with electron temperatures of about 2–3 keV. As a result of Z dependence analysis, several lines have been experimentally identified for the first time. Physical phenomena peculiar to highly charged heavy ions were clearly manifested, as described in the following sections.

2. Methods

The methods used in the LHD experiment are only briefly reviewed here since they have already been described in several previous papers [16,17,19,20]. In the LHD experiment, high-temperature (a few keV) and low-density (n_e = (3–5) $\times$ 10^{19} m^{-3}) hydrogen plasmas are routinely produced by several neutral beam injection (NBI) heating systems under a strong megnetic field of about 2.75 T. The plasma duration is typically 2–4 s, which is limited by the capability of the NBI heating. The electron temperature profiles are precisely measured by a Thomson scattering diagnostic system with high spatial and temporal resolution [24]. A small number (in the order of 10^{17} atoms) of heavy elements are injected into LHD plasmas using a tracer-encapsulated solid pellet (TESPEL) [25].

The temporal evolutions of EUV/soft X-ray spectra are recorded every 0.1 or 0.2 s, mainly by a 2 m Schwob–Fraenkel-type grazing incidence spectrometer called SOXMOS, equipped with a grating of 600 grooves/mm [26]. In addition, we also employed spectral data recorded by another grazing incidence spectrometer called EUV_Long, equipped with a flat field grating of 1200 grooves/mm [27]. The spectral resolutions of these spectrometers are 0.01–0.02 nm. The absolute wavelength is calibrated by using well-known lines of impurity ions such as carbon, neon, and iron. The uncertainty of the calibrated wavelength of the SOXMOS spectrometer is typically $\pm$0.005 nm.

As mentioned in the previous papers [17,19–21], discrete spectra due mainly to ions with 4s or 4p outermost electrons are observed in high-temperature conditions ($\simeq$1–3 keV). In contrast, quasi-continuum features (the so-called unresolved transition array) of ions with 4d or 4f outermost electrons are observed in low-temperature conditions (below 1 keV). In this study, therefore, we analyzed a series of discrete spectra recorded in high-temperature conditions as they include isolated lines of Ga-like ions.

The measured wavelengths are compared with those calculated by GRASP92 code, which employs the multi-configuration Dirac Fock (MCDF) method for precise atomic structure calculations [28]. In the GRASP92 code calculation, an atomic state function (ASF) is represented as a linear combination of multiple configuration state functions (CSFs). The single electron orbitals are optimized stepwise by increasing the number of CSFs until the calculated transition wavelengths are well converged. The detailed procedure for this optimization has already been described in our recent paper [29]. In addition, transition strengths are calculated with RATIP code from GRASP92 output [30]. However, the line intensities are not discussed in this article because the measured line intensity is not necessarily proportional to the calculated transition strength.

3. Results and Discussion

As mentioned in the introduction, EUV and soft X-ray spectra of Ga-like heavy ions are composed of a few isolated lines. Among them, we have already reported the wavelengths of the resonance transition from the level designated as $(4d_-)_{3/2}$ configuration in our recent paper [29], in which we clarified that the peculiar Z dependence of the transition wavelength is caused by strong Z-dependent mixing between the configurations $(4d_-)_{3/2}$ and

(4s, $(4p_+^2)_2)_{3/2}$. Therefore, this paper describes the other resonance transitions, including a magnetic dipole (M1) transition.

Figure 1 shows typical spectra of europium (Z = 63) ions in a high-temperature LHD plasma in the two different wavelength ranges measured simultaneously by SOXMOS spectrometer. The line broadening seen in Figure 1 mostly comes from the instrumental width due mainly to the spread of the electron bunch in the gap between a microchannel plate (MCP) and a phosphor screen. The other broadenings are considered to be negligible in comparison with the instrumental width. As indicated by a and b in Figure 1a, the resonance lines of the Ga-like ions are clearly seen adjacent to the intense resonance lines of the Cu-like and Zn-like ions indicated by square brackets. The lines a and b correspond to the allowed (E1) transitions from ((4s, $4p_-)_1$, $4p_+)_{3/2}$ and ((4s, $4p_-)_1$, $4p_+)_{1/2}$, respectively, to the ground state $(4p_-)_{1/2}$. In the longer wavelength range in Figure 1b, we found an intense line indicated by c at around 30.14 nm, which is identified as the M1 transition from $(4p_+)_{3/2}$.

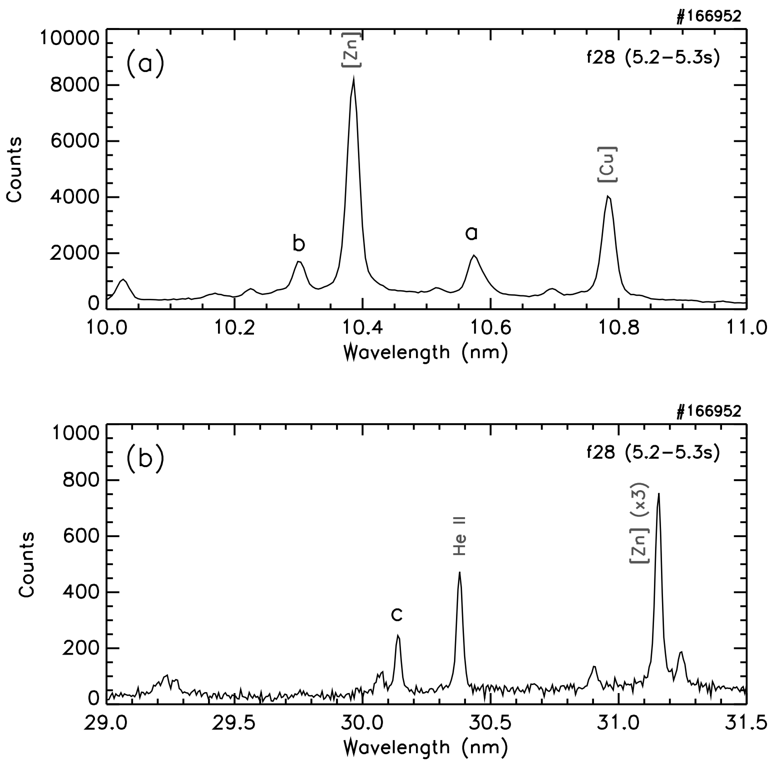

Figure 1. Spectra of europium (Z = 63) ions observed in high-temperature LHD plasmas in the wavelength ranges (**a**) 10–11 nm and (**b**) 29–31.5 nm, measured by the SOXMOS spectrometer. The lines a, b, and c are transitions of Ga-like ions from ((4s, $4p_-)_1$, $4p_+)_{3/2}$, ((4s, $4p_-)_1$, $4p_+)_{1/2}$, and $(4p_+)_{3/2}$, respectively, to the ground state $(4p_-)_{1/2}$. The lines of Cu-like and Zn-like europium ions are indicated by square brackets. The measured line broadening mostly comes from the instrumental width.

We have surveyed the existing spectral data observed in high-temperature LHD plasmas for Z from 57 onward to investigate Z dependencies of the wavelengths of these lines. Figure 2 shows the Z dependence of line a's observed wavelength (diamonds) together with theoretical wavelengths calculated by GRASP92 code (dotted line). The lines for Z = 60, 62, 64, 66, 68, and 70 could be easily identified because they have already been assigned in past experiments in NIST EBIT [10–14]. We predicted the wavelength for the other elements by the interpolation or extrapolation of Z dependence based on the past EBIT data, which resulted in the easier identification of the spectral lines. In contrast to the $(4d_-)_{3/2}$ configuration mentioned above, the effect of configuration mixing is considerably lower and very weakly dependent on Z for ((4s, $4p_-)_1$, $4p_+)_{3/2}$ and ((4s, $4p_-)_1$, $4p_+)_{1/2}$

configurations. Therefore, it is clearly shown that the Z dependence of the wavelength is lined up along a single smooth curve in the range of Z = 57–71. However, the theoretical wavelengths are slightly shorter than the measurements. This trend is also the case for line *b* except that the wavelengths are shifted to the shorter side of line *a*. Consequently, we have experimentally identified the lines for Z = 57–59, 63, 65, 67, 69, and 71 for the first time in this study.

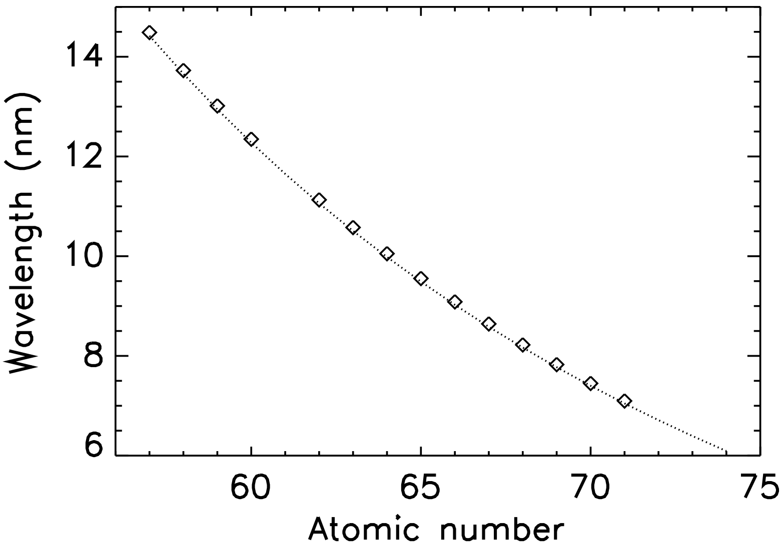

Figure 2. Z dependence of the transition wavelength from $((4s, 4p_-)_1, 4p_+)_{3/2}$ to the ground state (line *a* in Figure 1a) of Ga-like ions. The wavelengths measured in LHD plasmas are shown by diamonds, while the calculated wavelength is drawn by a dotted line.

Similarly, the Z dependence of the transition wavelength for line *c* in Figure 1b is plotted in Figure 3. As is well known, this forbidden line corresponds to the M1 transition between the levels split by the spin–orbit interaction of the ground state configuration [Ar]$3d^{10}4s^24p$. In general, the energy splitting due to the spin–orbit interaction rapidly increases with Z. For example, the Hamiltonian of the spin–orbit interaction for a hydrogen-like system is proportional to the fourth power of Z. Therefore, the wavelengths corresponding to this energy splitting are in the EUV range due to the large spin–orbit interaction for heavy ions. Again, the wavelengths measured in the LHD are indicated by diamonds, while a dotted line plots the calculated wavelength. Though the measured wavelengths for Z less than 63 are missing because of the limited wavelength range of the spectrometers used in this study, the calculated wavelength is given in the entire range of Z. We took the measured wavelength for tungsten (Z = 74) from our previous paper [2]. Though the wavelength of the M1 line for ytterbium (Z = 70) has also been reported recently in NIST EBIT [14], the M1 lines for the other elements (Z = 63–69 and 71) have been identified experimentally for the first time in this study. As shown in Figure 3, the experimental wavelengths of the M1 transition are in very good agreement with the calculated ones.

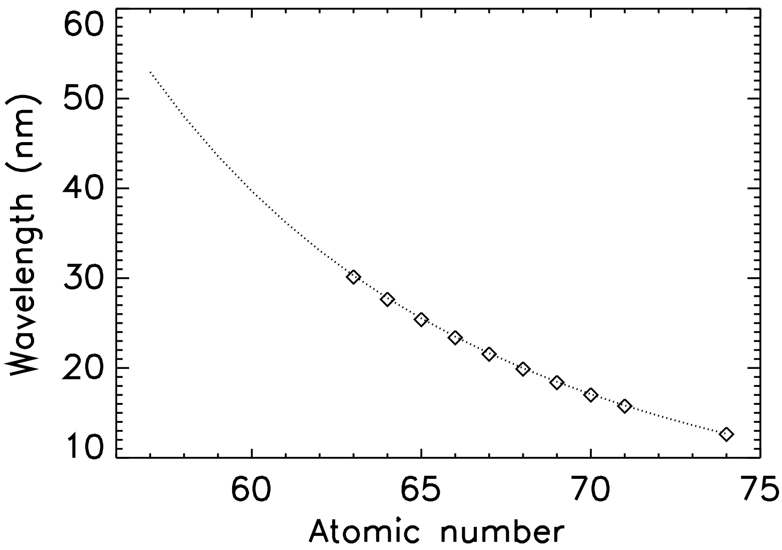

Figure 3. Z dependence of the wavelength of the magnetic dipole (M1) transition from $(4p_+)_{3/2}$ to the ground state (line *c* in Figure 1b) of Ga-like ions. The wavelengths measured in LHD plasmas are shown by diamonds, while the calculated wavelength is drawn by a dotted line.

4. Summary

We have analyzed the EUV/soft X-ray emission spectra of Ga-like heavy ions observed in high-temperature LHD plasmas. A number of prominent lines of Ga-like ions, including M1 transitions between doublets of the ground state configuration, have been assigned experimentally for the first time in LHD from the analyses of Z dependencies. The measured wavelengths are in good agreement with the theoretical values calculated with an MCDF code GRASP92. We have confirmed that the results reflect the large effects of the Z-dependent configuration interaction and spin–orbit interaction, which are physical properties specific to highly charged heavy ions. As the analyses based on the comparisons with theories and other experiments are still underway, the detailed comparisons and interpretations of the Z dependencies will be reported in a separate paper in the near future.

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