Temperature Dependent Shape of Quasi-Continuum Spectra from Highly Charged Heavy Ions Observed in the Large Helical Device*)

Chihiro SUZUKI[1,2], Fumihiro KOIKE[3], Izumi MURAKAMI[1,2] and Naoki TAMURA[1]

[1] *National Institute for Fusion Science, National Institutes of Natural Sciences, Toki 509-5292, Japan*
[2] *The Graduate University for Advanced Studies, SOKENDAI, Toki 509-5292, Japan*
[3] *Department of Materials and Life Sciences, Sophia University, Tokyo 102-8554, Japan*

(Received 24 July 2024 / Accepted 20 September 2024)

The temperature dependent shape of quasi-continuum unresolved transition array (UTA) spectra from highly charged heavy ions has been examined based on the experimental spectra recorded in the Large Helical Device plasmas. The observed spectral shape of the n=4–4 UTA emission strongly depends on the electron temperature especially for the lanthanide elements with the atomic numbers of 63 - 66. As the temperature decreases, the UTA position moves to shorter wavelength and the UTA bandwidth becomes narrower. Eventually, characteristic narrowed spectra with the lines of palladium-like and silver-like ions are observed at the lowest peak temperature of a few hundred eV. The temperature dependence of the UTA shape can be explained by the change in ion abundance and the wavelength distributions of the weighted transition probabilities calculated with the Flexible Atomic Code (FAC). A collisional-radiative modeling of the narrowed spectrum for terbium ions is tried based on the FLYCHK code and the FAC. As a result of slight intentional shifts of the calculated line positions, the measured spectrum matches qualitatively with the simulation for the electron temperature of 230 eV.

Keywords: highly charged ions, soft X-ray spectroscopy, UTA, LHD, lanthanides, FAC, FLYCHK, collisional-radiative model

DOI: 10.1585/pfr.20.2401006

1. Introduction

It is well known that the emission spectra from highly charged heavy ions often appear in the extreme ultraviolet (EUV) and soft X-ray regions as quasi-continuum bands composed of a huge number of lines [1]. The extremely complex energy level structure of a heavy ion with partially filled orbitals of high angular momentum (e.g., $4d^5$, $4f^7$) leads to the quasi-continuum band in which the average line interval is smaller than each line broadening. In this sense, such a quasi-continuum band is often referred to as unresolved transition array (UTA) [2]. In particular, the UTAs arising from n=4–4 transitions of ions with outermost 4d or 4f subshell are outstanding because spectra from a wide range of charge states are overlapped in the same spectral region.

We have so far observed various UTA spectra from highly charged heavy ions in the Large Helical Device (LHD), a magnetically confined torus plasma device at the National Institute for Fusion Science (NIFS). A variety of heavy elements with the atomic numbers (Z) of 50 - 83 have been systematically investigated in the last decades [3–5]. The observed spectral shape of the n=4–4 UTA emission strongly depends on the electron temperature for some of the lanthanide elements. In this study, we present a qualitative interpretation of this temperature dependent spectral shape based on the comparisons with the calculated wavelength distributions of the weighted transition probabilities. In addition, we try to simulate a characteristic narrowed spectral shape observed in a low-temperature (<500 eV) condition using a collisional-radiative (CR) model.

2. Experimental

All the experimental data used in this study were recorded in the LHD plasmas with the injection of heavy elements as an impurity. The heavy elements are introduced into high-temperature (≃2 - 3 keV) hydrogen plasmas using a tracer encapsulated solid pellet (TESPEL) [6]. The EUV and soft X-ray spectra used in this study were measured by a 2 m grazing incidence spectrometer called SOXMOS with a 600 grooves/mm grating [7]. The wavelength is calibrated with an uncertainty of ±0.003 nm using a polynomial fitting of well-known lines of various impurity ions. We observed the line-integrated spectra along the line of sight adjusted to the path through the plasma center. The spectral resolution is approximately 0.01 nm which is enough to discuss the shape of UTA although a line shape of a single line is unresolvable. The spectra are sequentially recorded every 100 ms while the plasma is maintained for several seconds. Therefore, the spectra for various electron temperatures can be measured in a sin-

author's e-mail: csuzuki@nifs.ac.jp
*) This article is based on the presentation at the 26th International Conference on Spectral Line Shapes (ICSLS2024).

gle discharge by changing the heating power. The electron temperature and density profiles are measured by an existing Thomson scattering diagnostic system with high spatial and temporal resolutions [8].

3. Temperature Dependence

The temperature dependence of the observed quasi-continuum UTA shape was particularly outstanding for the lanthanide elements with Z of 63 - 66. For example, Fig. 1 shows three different soft X-ray spectra of terbium (Tb: Z=65) ions measured in a single discharge. The peak electron temperature for each spectrum is also displayed in Fig. 1. Figure 2 shows temporal evolutions of heating power, line-averaged electron density and electron temperature in the same discharge as in Fig. 1. Electron temperatures at the center and at 0.45 m in the effective minor radius are plotted in Fig. 2 (c). A TESPEL containing Tb powder was injected at 3.8 s during the neutral beam injection (NBI) heating to keep high electron temperature around 2 keV in the core. The heating power was dropped at 4.4 s due to the extinction of NBI #2, which triggered a rapid decrease in core electron temperature. The UTA spectra in Fig. 1 were measured sequentially in this period (4.4 - 4.7 s). In Fig. 1 (c), a hollow temperature profile (so-called "temperature hole") [4] is formed as the temperature is zero in the core and have a peak of about 300 eV in the outer region as shown in Fig. 2 (c).

Figure 1 clearly illustrates that the position and the shape of the UTA largely change with the electron temperature. As the temperature decreases, the peak position moves to shorter wavelength side while the width becomes narrower. Eventually, a narrowed band emission with a strong peak at 6.514 nm appears as shown in Fig. 1 (c).

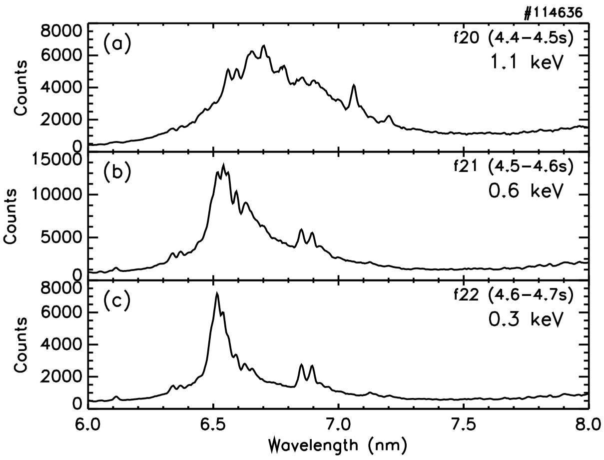

Fig. 1 Soft X-ray spectra of terbium (Tb) ions observed in an LHD plasma (shot number #114636) with a TESPEL injection. Three different spectra for peak electron temperatures of (a) 1.1 keV, (b) 0.6 keV and (c) 0.3 keV are plotted. The number and period for each time frame are also indicated.

This narrowed spectrum looks slightly asymmetric with a tail in longer wavelength side, which is characterized by a remarkable doublet peak at 6.851 and 6.895 nm. The main peak and the doublet peak are assigned to the emission lines of palladium-like (Pd-like) Tb^{19+} and silver-like (Ag-like) Tb^{18+} ions, respectively, because the wavelengths of these peaks are in excellent agreement with the past experimental values [9, 10].

This temperature dependent shape of the quasi-continuum spectrum is attributable to the change in dominant charge states in the plasma. Figure 3 shows the wavelength distributions of the weighted transition probabil-

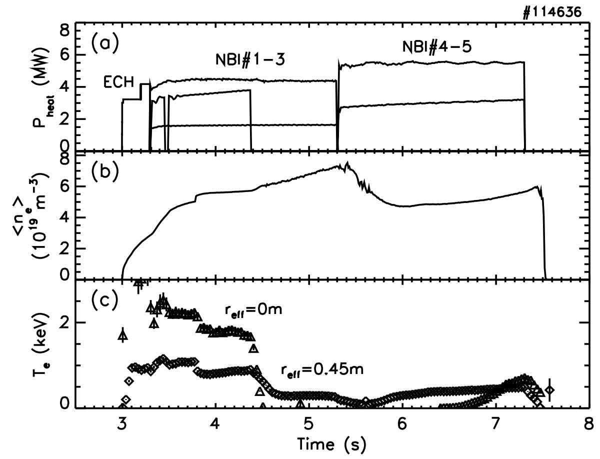

Fig. 2 Temporal evolutions of (a) heating power P_{heat}, (b) line-averaged electron density $<n_e>$ and (c) electron temperature T_e in the same plasma as in Fig. 1. Electron temperatures at the center and at 0.45 m in the effective minor radius are plotted in (c).

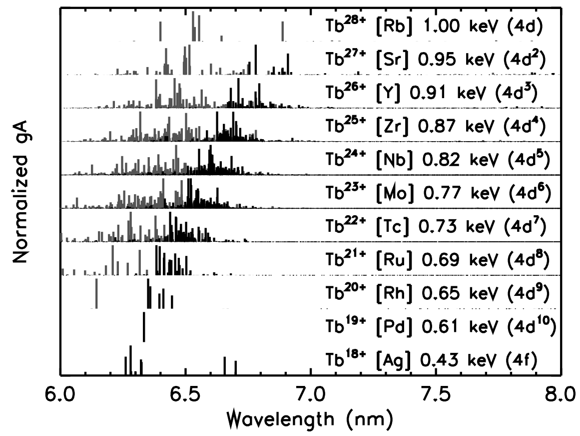

Fig. 3 Calculated wavelength distributions of the weighted transition probability (gA) for 4d-4f (black) and 4p-4d (grey) transitions of Tb ions. The intensities for charge states from Rb-like (Tb^{28+}) to Ag-like (Tb^{18+}) isoelectronic sequences are shown. The intensities are normalized for each charge state and transition type. The ionization energy and the ground state configuration for each charge state are also indicated.

ity (gA) of n=4–4 transitions for rubidium-like (Rb-like) Tb^{28+} to Ag-like Tb^{18+} ions, calculated with the Flexible Atomic Code (FAC) in which the atomic structure is calculated using Multi-configuration Dirac-Fock method with local potential approximation [11]. The gA intensities plotted in Fig. 3 are normalized for each charge state and transition type. It is clearly seen that the mean position of the line group moves to shorter wavelength as the ion charge decreases. This trend is qualitatively consistent with the observed spectra in Fig. 1 because the fractional ion abundance should move to lower charge as the electron temperature decreases. The calculation also implies that the narrowed spectrum in Fig. 1 (c) would largely originate from Pd-like and Ag-like ions because the main and doublet peaks are seen in the calculation for these ions. The spectral feature for these ions look relatively simple rather than quasi-continuum because the 4d orbital is nearly closed.

We have also surveyed thoroughly the Z dependence of the narrowed spectrum in the low-temperature condition for all the lanthanide elements except for Z=61. The position and shape of the spectrum gradually change with Z. The mean position of the narrowed spectrum moves to shorter wavelength with increasing Z. The narrowed spectrum accompanied with the clear peaks of Pd-like and Ag-like ions is remarkably outstanding in Z=63 - 66. The doublet peak of Ag-like ions disappear for Z lower than 63, while the bandwidth of the main UTA is gradually broadened as Z increases beyond 66.

4. Simulation of the Narrowed Spectrum

In this section we focus on the characteristic narrowed spectrum of Tb ions shown in Fig. 1 (c). When this spectrum was observed, the temperature hole was formed as mentioned in Sec. 3. Judging from the Thomson scattering diagnostic data, the emission should originate from the outside region where the density is $(2 - 15)\times10^{19}$ m^{-3} and the temperature is lower than 350 eV.

The discussion in Sec. 3 implies that a few charge states around Pd-like ion are dominant in this condition. In order to simulate the measured spectrum, we tried to roughly estimate the fractional abundance in the emitting region using the FLYCHK code based on a non-LTE (non-local thermodynamic equilibrium) model under hydrogenic approximation [12]. The density dependence can be ignored here because the average charge calculated as a function of temperature remains almost unchanged in the density range of 10^{18} - 10^{20} m^{-3}. The temperature dependence of the fractional abundance of Tb ions is plotted in Fig. 4 in which three charge states, Ag-like, Pd-like and rhodium-like (Rh-like) ions, are emphasized by thick black lines. It indicates that these charge states would be dominant in the temperature range of 200 - 300 eV, which is consistent with the discussion in Sec. 3.

Next we try to reproduce the narrowed spectrum us-

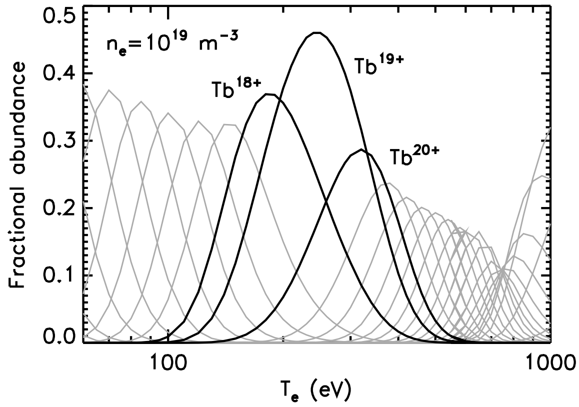

Fig. 4 Fractional ion abundance of Tb ions calculated by FLYCHK code as a function of electron temperature. Electron density is assumed to be 10^{19} m^{-3}.

ing the CR model included in the FAC. For simplicity, we only considered three charge states (Tb^{18+}–Tb^{20+}) mentioned above. The calculation only includes single electron excited configurations up to n=5, and the CR model only includes spontaneous emission and electron impact excitation/de-excitation to reduce the calculation time for the cross sections of elementary processes. Also, single temperature is assumed, that is, the effect of line integration along the line of sight is ignored.

For a comparison with the experiment, the calculated spectra for the three charge states need to be synthesized with the fractional abundance estimated by the FLYCHK code. However, it should be noted here that the calculated wavelengths of the identified lines of Pd-like and Ag-like ions systematically deviate approximately 0.2 nm to shorter wavelength side. For example, the calculated wavelength for the $4d^{10}\ {}^1S_0$–$4d^9 4f\ {}^1P_1$ transition of Pd-like Tb^{19+} ion is 6.334 nm, while the experimental wavelength of this line in LHD is 6.514 nm. This indicates that the calculated spectra need to be slightly shifted so as to meet the experimental spectra. Therefore, the calculated spectra for Ag-like and Pd-like ions were shifted by 0.195 and 0.180 nm to longer wavelength side, respectively, based on the measured values in LHD. As for Rh-like ion, the appropriate value of the shift is unknown because no lines are identified. In this study, we assumed the shift for Rh-like ion is the same as that for Pd-like ion. We synthesized the shifted three spectra with the weight determined by the calculated fractional abundance.

Consequently, we obtained the simulated spectra for the temperature range of 200 - 300 eV. For example, the simulated spectrum at 230 eV is shown in Fig. 5 together with the measured spectrum (same as Fig. 1 (c)). The overall feature of the narrowed spectral shape qualitatively matches with the simulation for 230 eV except for the fine details. It is noted that there still remains weak background quasi-continuum feature in the observed spectrum, which

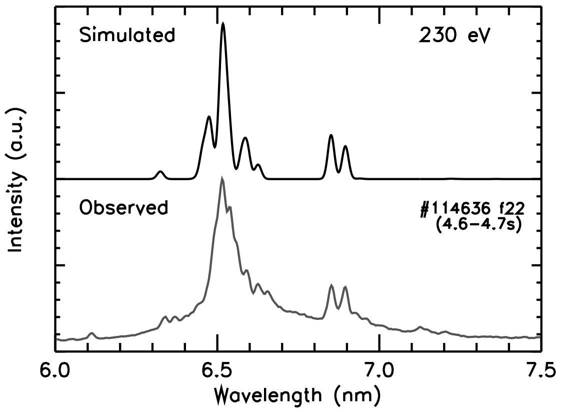

Fig. 5 The simulated (top) and the observed (bottom) spectra of Tb ions. The simulated spectra are slightly shifted to longer wavelengths before synthesizing the spectra for three charge states. The observed spectrum is the same as Fig. 1 (c).

may originate from broad UTAs of the other charge states as suggested from the gA distributions shown in Fig. 3.

5. Summary

In LHD plasmas, we have systematically observed soft X-ray spectra of n=4–4 transitions of highly charged heavy ions. Temperature dependent shape of quasi-continuum UTA spectra can be qualitatively explained by the calculated line positions for ions with outermost 4d subshell. The narrowed spectral shape outstanding in Z=63 - 66 is mainly composed of a few charge states around Pd-like ion, and is qualitatively simulated by the CR model for three ion stages if the calculated wavelengths are intentionally shifted by approximately 0.2 nm.

Acknowledgments

The authors acknowledge the continuing support from the LHD experiment group members. This work was carried out with the support and under the auspices of the NIFS collaboration research program (NIFS22KIIF003). This work was supported also by JSPS KAKENHI Grant Numbers 21K03515 and 21H04460.

[1] G. O'Sullivan and P.K. Carroll, J. Opt. Soc. Am. **71**, 227 (1981).
[2] J. Bauche *et al.*, Phys. Scr. **37**, 659 (1988).
[3] C. Suzuki *et al.*, J. Phys. B: At. Mol. Opt. Phys. **48**, 144012 (2015).
[4] C. Suzuki *et al.*, Plasma Phys. Control. Fusion **59**, 014009 (2017).
[5] C. Suzuki *et al.*, Atoms **6**, 24 (2018).
[6] S. Sudo and N. Tamura, Rev. Sci. Instrum. **83**, 023503 (2012).
[7] J.L. Schwob *et al.*, Rev. Sci. Instrum. **58**, 1601 (1987).
[8] I. Yamada *et al.*, Rev. Sci. Instrum. **81**, 10D522 (2010).
[9] J. Sugar *et al.*, J. Opt. Soc. Am. B **10**, 799 (1993).
[10] J. Sugar *et al.*, J. Opt. Soc. Am. B **10**, 1321 (1993).
[11] M.F. Gu, Can. J. Phys. **86**, 675 (2008).
[12] H.-K. Chung *et al.*, High Energy Density Phys. **1**, 3 (2005).