High Energy Density Physics 20 (2016) 17–22

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Model uncertainties of local-thermodynamic-equilibrium K-shell spectroscopy

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ARTICLE INFO

Article history:
Received 29 February 2016
Received in revised form 23 May 2016
Accepted 30 May 2016
Available online 6 June 2016

Keywords:
X-ray spectroscopy
Plasma diagnostics
LTE
Opacity
Diagnostics uncertainty
Line shape

ABSTRACT

Local-thermodynamic-equilibrium (LTE) K-shell spectroscopy is a common tool to diagnose electron density, n_e, and electron temperature, T_e, of high-energy-density (HED) plasmas. Knowing the accuracy of such diagnostics is important to provide quantitative conclusions of many HED-plasma research efforts. For example, Fe opacities were recently measured at multiple conditions at the Sandia National Laboratories Z machine (Bailey et al., 2015), showing significant disagreement with modeled opacities. Since the plasma conditions were measured using K-shell spectroscopy of tracer Mg (Nagayama et al., 2014), one concern is the accuracy of the inferred Fe conditions. In this article, we investigate the K-shell spectroscopy model uncertainties by analyzing the Mg spectra computed with 11 different models at the same conditions. We find that the inferred conditions differ by ±20–30% in n_e and ±2–4% in T_e depending on the choice of spectral model. Also, we find that half of the T_e uncertainty comes from n_e uncertainty. To refine the accuracy of the K-shell spectroscopy, it is important to scrutinize and experimentally validate line-shape theory. We investigate the impact of the inferred n_e and T_e model uncertainty on the Fe opacity measurements. Its impact is small and does not explain the reported discrepancies.

1. Introduction

In high-energy-density (HED) plasmas, emergent K-shell spectral lines are sensitive to electron density, n_e, and electron temperature, T_e, of the source plasma [1–5]. The spectral line shapes strongly depend on n_e via Stark line broadening. The ratios of spectral lines from adjacent charge states are very sensitive to T_e. K-shell spectroscopy is considered well understood and is a common tool to diagnose n_e and T_e of HED plasmas.

We recently measured Fe opacity at multiple conditions relevant to the solar interior and revealed 30–400% disagreement with modeled Fe opacities [6]. The n_e and T_e of those measurements were determined with K-shell spectroscopy of tracer Mg [5]. One may question the accuracy of these inferred conditions. While the reported measurement uncertainties included experiment-to-experiment reproducibility and fit uncertainties due to noise, they did not include all the uncertainties associated with the analysis method itself. For example, the noise in the data can affect not only the fit but also some intermediate processing steps such as the continuum-baseline determination discussed in Ref. 5. Also, the measured absorption lines are saturated to some extent due to the instrumental broadening. To minimize those concerns, we avoided heavily saturated lines in the analysis and accounted for the instrumental broadening effects on the modeled spectra. However, the instrumental broadening does slightly reduce the diagnostic sensitivity, and this contribution should be assessed. Perhaps the most important uncertainty neglected in Ref. 5 is that associated with potential inaccuracy of the spectral model. Validating spectral models requires dedicated experiments and is beyond the scope of this work,

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http://dx.doi.org/10.1016/j.hedp.2016.05.001
1574-1818/

but we can at least investigate how much difference in n_e and T_e arises if different spectral models are used in the interpretation.

In this article, we quantify the uncertainties of inferred n_e and T_e due to the analysis method and the choice of spectral model through analyses of synthetic data. We first verify that the analysis method accurately infers conditions within 2σ of the fit uncertainty even when accounting for noise and the saturation due to the instrumental broadening. Then, we investigate the K-shell spectroscopy model uncertainty by analyzing Mg K-shell spectra calculated with 11 different models at the conditions relevant to the Fe opacity experiments [5]. We find that the inferred conditions can vary by ±20–30% in n_e and ±2–4% in T_e depending on the choice of spectral model. This significant n_e discrepancy originates from differences in the line-shape calculations in the spectral models. Since n_e affects the charge-state distributions, this ±20–30% n_e uncertainty is also responsible for half of the T_e uncertainty. It is crucial to use accurate line-shape models for reliable K-shell spectroscopic diagnosis. Theoretical scrutiny and experimental validation of these line-shape models are essential for refining our understanding of HED plasmas. We further investigate the impact of these n_e and T_e uncertainties on the reported Fe opacity discrepancies and confirm they do not explain the major discrepancy.

The paper is organized as follows. Our investigation method and the synthetic data creation method are discussed in Sec. 2. We investigate the potential inaccuracy of our analysis method due to noise, instrumental broadening, and continuum-baseline determination in Sec. 3. Then, we numerically investigate the inferred-condition dependence on the spectral model in Sec. 4. Potential sources of the discrepancies are discussed in Sec. 5. The impact of the n_e and T_e uncertainty due to the spectral model dependence on the recent Fe opacity measurement is discussed in Sec. 6, and the conclusions are given in Sec. 7.

2. Synthetic data creation

To create various synthetic data, Mg K-shell opacity spectra are computed with 8 different models: ABAKO [7], ATOMIC [8,9], FLYCHK [10], OPAL [11], OPAS [12,13], PrismSPECT [14], SCO-RCG [15], and SCRAM [16]. Multiple calculations are submitted from some models with different line-shape calculation options or with different atomic-structure calculation options. As a result, there are a total of 11 different calculations for each condition. The spectra are computed at 1) $n_e = 0.9\times10^{22}$ cm^{-3} and $T_e = 165$ eV, and 2) $n_e = 4.0\times10^{22}$ cm^{-3} and $T_e = 195$ eV, which are similar to the conditions achieved by the recent Fe opacity measurements [5,6]. We remind the reader that we observed agreement between modeled and measured Fe opacities at the lower n_e and T_e conditions [17], while significant disagreement was found at the higher n_e and T_e case [6].

Synthetic data are computed from calculated opacities as follows. First, opacity spectra are converted to transmission spectra by:

$$T_\nu^{\text{modeled}} = \exp\left(-\rho L \kappa_\nu^{\text{modeled}}\right), \tag{1}$$

where κ_ν is the calculated opacity in cm^2/g, and ρL is typical Mg areal density used in our experiments. We use 3.0×10^{-5} and 4.9×10^{-5} g/cm^2 for each case. Second, we convolve transmission with instrumental broadening:

$$T_\nu^{\text{instrum}} = \int g(\nu-\nu') T_{\nu'}^{\text{modeled}} d\nu', \tag{2}$$

where $g(\nu-\nu')$ is the measured spectral resolution [18] of our spectrometers [4]. Then, a few-percent Poisson noise (i.e., typical in our measurements) is added to the spectra. We extract n_e and T_e from these synthetic data using the analysis method discussed in Ref. 5, permitting us to investigate the accuracy of our analysis method.

3. Analysis method accuracy

There are several concerns in the accuracy of the analysis discussed in Ref. 5. First, bound–bound (b–b) line transmission spectra were extracted from the measured absorption spectra by defining a smooth continuum baseline from the measured absorption spectra and dividing the spectra by this baseline [5]. The motivation behind this was that the spectral range where Mg K-shell lines appear also had significant Fe bound-free (b-f) continuum absorption. Since it was impossible to separate Mg b-f from the Fe b-f absorption and n_e and T_e sensitivities exist in the Mg b–b lines, we extracted Mg b–b line transmission spectra for n_e and T_e analysis. Since Mg b–b lines were well isolated, it was rather straightforward to define the baseline. However, it is always a concern how the noise in the data can affect the baseline determination and the analysis results. Second, for efficient analysis, we construct a Mg opacity database using PrismSPECT [14] with detailed line shapes computed with MERL [19,20]. A genetic algorithm followed by a Levenberg–Marquardt non-linear least-squares minimization method [21] interpolates the database and searches for the optimal n_e and T_e to reproduce the data. A concern is whether or not the analysis based on the database with linear interpolation provides sufficiently accurate results. Finally, we would like to know how accurately we can infer n_e and T_e from lines that are partially saturated due to instrumental broadening. To minimize errors associated with this complexity, we measured spectra with an instrument with high resolving power ($E/\Delta E \approx 900$), use only weaker lines in the analysis, and take into account the instrumental broadening in the modeled transmission spectra. However, it is still not clear how accurately n_e can be inferred from altered line shapes because density sensitivity must be somewhat reduced.

We can test potential analysis inaccuracy due to the above limitations by comparing the target conditions with the conditions inferred from the synthetic data, which are directly computed with PrismSPECT with the MERL line shapes. Red lines in Fig. 1 are the b–b line transmission spectra extracted from the PrismSPECT synthetic data. They are computed at (a) $n_e = 0.9\times10^{22}$ cm^{-3} and $T_e = 165$ eV, and (b) $n_e = 4.0\times10^{22}$ cm^{-3} and $T_e = 195$ eV. To minimize the saturation effects on the analysis, we analyze weaker lines whose optical depths are $\lesssim$1.0: Lyα, Heγ, Heδ, and Lyβ at the lower n_e, and T_e case, and Heγ and Lyβ at the higher n_e and T_e case. Fig. 2 shows the results of the chi-square fit of the diagnostic lines. The reduced χ^2 is close to unity, quantitatively confirming the goodness of the fit. The conditions inferred by the fit-optimization are (a) $n_e = (0.95\pm0.04)\times10^{22}$ cm^{-3} and $T_e = 166\pm1$ eV, and (b) $n_e = (4.2\pm0.1)\times10^{22}$ cm^{-3} and $T_e = 195\pm1$ eV. These agree with the target conditions that are used to create the synthetic data within 2σ and 1σ of the fit uncertainty, respectively. This confirms that the analysis method using the selected lines still infers conditions accurately within ± 5% in n_e and ± 1% in T_e even while accounting for noise and the small line saturation due to instrumental broadening.

4. Spectral-model uncertainty

For each condition, 11 synthetic spectra computed with different models (Sec. 2) are analyzed using the Mg opacity database constructed with PrismSPECT and MERL and the methods discussed in Sec. 3. Since the same analysis method is employed, the standard deviation in the inferred conditions represents the uncertainties due to the spectral-model differences.

Fig. 3 shows n_e (left) and T_e (right) inferred from synthetic data computed with different models, plotted in percent difference from the mean. The diagnostic uncertainties due to the spectral models are (a) $\Delta n_e = \pm 19\%$ and $\Delta T_e = \pm 2.0\%$ at the lower n_e and T_e case, and (b) $\Delta n_e = \pm 24\%$ and $\Delta T_e = \pm 3.5\%$ at the higher n_e and T_e case, which are more significant than those due to the analysis method (Sec. 3).