Laser-produced molybdenum plasma analysis with a Collisional - Radiative model included in the hydrodynamic code med103

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Abstract. The Collisional-Radiative (CR) model with fine atomic data included in the hydrodynamic code MED103 is used for the soft x-ray spectra analysis of laser-produced molybdenum plasmas. The charge distribution drawn from the soft x-ray spectra can be used to determine the pre-plasma conditions for the plasma-based molybdenum soft x-ray lasers (SXRLs).

1. Introduction

X-ray spectroscopy is a powerful tool in the study of plasmas both in the universe and the laboratory. The laboratory plasmas generated by high intense lasers, z-pinch machines and tokamak devices, etc., usually have quite different conditions. Such complicated plasmas impose high requirements on the theoretical analysis of the spectra recorded with various spectrometers equipped with gratings or crystals. In order to extract the physics underlying the phenomenon from the recorded spectrographs, one usually turns to certain radiation-hydrodynamics codes. The Collisional-Radiative model (CR model) has been proven as the most successful model to analyze the laboratory plasma which is usually in non-local thermodynamic equilibrium (non-LTE). Much work has been done in the development of various codes with CR model, for the wide range of applications in plasma experimental design and spectral analysis [1]. International workshops on non-LTE kinetics have led to a significant progress on the CR models and hence to a better agreement with well characterized measurements [2].

In this paper, we present the application of the Collisional-Radiative (CR) model code on the analysis of laser-produced Molybdenum plasmas. By comparing the calculated soft x-ray spectra with that measured in experiments, it is able to deduce the charge distribution of the laser-produced plasmas, and the contributions of different physical process can also be obtained with further detailed analysis.

2. Experiments

The experiment was carried out on the XL-II Ti:sapphire laser facility at the Institute of Physics, Chinese Academy of Sciences. The laser typically delivers pulses of energy about 500 mJ in 200 picoseconds with central wavelength at 800nm. The uncompressed beam was directed into the target
chamber and focused onto a molybdenum slab target using a single $f/8$ spherical lens. By adjusting the lens position from the target we could vary the focal spot size from tens to hundreds of micrometers monitored by a cross-slit camera filtered with 1.2 μm thickness aluminum. The x-ray image was recorded on a back-illuminated CCD. In some shots, a serial of neutral density filters were inserted into the beam path to change the laser energy focused on the target, so that the difference of the two intensity-changing methods could also be studied. The plasma x-ray emission was observed 45° off the target normal by using an on-axis flat field spectrometer equipped with a Hitachi 1200 lines/mm variably spaced spherical grating, which was located 321 mm from the target and set to a grazing angle of 3°. Another 2048 × 512 pixel, back-illuminated CCD camera was coupled to the focal plane of the grating to record the spectrograph. Figure 1 shows the typical corrected on-axis spectra of the plasma created by a 400-mJ laser pulse with the average intensity of $3.5 \times 10^{15}$ W/cm$^2$. The well-resolved line is imposed on a strong recombination continuum emission.

3. Data Analysis

3.1.1. Calibration and spectra intensity correction of CCD camera

A long-year-used CCD camera usually has the layer of silicon oxide grown on the silicon surface and the dead layer, which affect the quantum efficiency QE dramatically and trouble the spectra analysis in the soft x-ray region. We calibrated our CCD camera by using the method of Li’s [3].

The interaction efficiency of a CCD can be written as

$$\eta_{\text{int}}(\lambda) = \exp\left[-\alpha_{\text{ox}}(\lambda)t_{\text{ox}}\right] \times \left[1 - \exp\left[-\alpha(\lambda)t\right]\right],$$

where $t$ and $t_{\text{ox}}$ are the thickness of the active region and that of the oxide layer. $\alpha$ and $\alpha_{\text{ox}}$ are the related absorption coefficients [4].

The reflectivity of the surface is neglected. The collection efficiency is

$$\eta_{\text{coll}}(\lambda) = \exp\left[-\alpha(\lambda)t_{\text{d}}\right],$$

with $t_{\text{d}}$ the thickness of the dead layer.

The quantum efficiency QE of the device is the production of the two above, i.e.,

$$QE(\lambda) = \eta_{\text{int}}(\lambda)\eta_{\text{coll}}(\lambda).$$

With this semi-empirical method we can get the calculated quantum efficiency curves by simply assuming the layer thickness then comparing the silicon L-edge jump with the experiment spectra to find the fitted thickness for the QE. In the data correction we used $t_{\text{ox}} = 10 \text{ nm}$, $t = 10 \text{ μm}$ and $t_{\text{d}} = 30 \text{ nm}$.

The calculated QE can be taken as the semi-empirical calibration of the CCD camera with which we corrected the spectrograph of the molybdenum plasma emissions in soft x-ray region 8nm ~ 22nm, shown as the red line in Figure 1.

3.1.2. Theoretical Model

To investigate the physical progress, the Collisional-Radiative (CR) model was employed to simulate the results by using the same laser conditions with the experiment. In the Collisional-Radiative model, atomic level populations are calculated by solving multi-level atomic rate equations self-consistently, which is a complicated and time-consuming progress. For the molybdenum simulation 1579 levels from Mo9 to Mo15 was used, the others were treated as H-like. The model considers important atomic processes and their inverse processes: collisional excitation and deexcitation for radiationless bound-bound transitions, collisional ionization and recombination, autoionization and electron capture. For radiative process, the code includes the spontaneous emission for bound-bound transitions and the radiative recombination, while an escape factor is introduced for the re-absorption of the emission instead of considering the photo-excitation and the photo-ionization processes, since there is no
external field applied in the experiments except the laser pulse. In the model the time dependent rate equations are resolved within the hydro code.

The rates of the collisional excitation and the de-excitation are from the method of van Wyngaarden et al. [5] with the collision strength calculated with the Cowan code [6]. The collisional ionization rate is calculated with Lotz’s [7] model. The rate coefficient from an ion i to ion i+1 is given by

$$R_{i,i+1}/N_e = 2.97 \times 10^{-6} \left( \frac{\xi}{I_n \sqrt{T_e}} \right) E_i(U),$$

where \(\xi\) is the number of electrons in the outer shell of the ion being ionized. \(I_n\) is the ionization potential of the shell in eV. The \(E_i\) is the exponential integral of the first kind with \(U = I_n/T_e\). For a Maxwellian electron distribution, the collisional recombination is calculated according to the principle of detail balance:

$$R_{i,i+1}/N_e = 1.66 \times 10^{-22} \left( \frac{g_i}{g_{i+1}} \right) \left( \frac{e^{U/T_e}}{T_e^{3/2}} \right) R_{i,i+1},$$

where \(g_i\) and \(g_{i+1}\) are the statistical weights of the respective states and \(R_{i,i+1}\) is the ionization rate coefficient.

In laser-generated molybdenum plasmas, strong continuum emission due to the recombinations was observed to dominate in measured soft x-ray range. The atomic process contributes to the continuum emission is the radiative recombination. The rate is given by

$$R_{i,i+1} = \left( \frac{n_i}{n_{i+1}} \right)^* 4 \pi \int_0^{\infty} \alpha_{i,i+1} \left( \frac{2h\nu^3}{c^2} \right) e^{-h\nu/kT_e} \frac{dv}{h\nu}$$

The \((n_i/n_{i+1})^*\) given by the Saha-Boltzmann equation

$$\left( \frac{n_i}{n_{i+1}} \right)^* = 1.66 \times 10^{-22} \left( \frac{g_i}{g_{i+1}} \right) \left( \frac{e^{U/T_e}}{T_e^{3/2}} \right).$$

The \(\alpha_{i,i+1}\) is the radiative recombination cross-section for the species of interest, which assumed given by the hydrogenic formula allowing for the non-hydrogenic ionization potential, \(I_n\), of the ion of charge \(Z\), i.e.

$$\alpha_{i,i+1} = 4.12 \times 10^{-26} \left( \frac{I_n^{5/2}}{Z} \right) (1/\nu^3)$$

Figure 1. Comparison of the Mo plasma spectra recorded with CCD corrected by detector response and simulated one with CR model code.

Figure 2. Charge state fraction of the average ionization stage between the electron density of 5×10^{19} cm^{-3} and 5×10^{20} cm^{-3} from the hydrodynamic code MED103.
To investigate the physical progress from the spectra of molybdenum plasmas, we did the CR model simulation using the same experiment laser conditions of $3.5 \times 10^{12}$ W/cm², also the results are time-integrated and space-integrated as in the experiments. The comparison of the measured spectra after semi-empirical calibration, and the synthetic one calculated with CR model, is shown in Figure 1. A good recombination continuum shape agreement is seen over the whole wavelength scale. However, the intensity at both wings of the spectra does not match with the measurement quite well. The intensity mismatch at the wings of Figure 1 might be caused by the fact that the experiment has a Gaussian laser intensity distribution at the focus, while the numerical simulations assume only a single intensity. Furthermore, for a long distance transfer the wave front cannot be the perfect Gaussian shape anymore, which means the spectrum recorded in our experiment might come from sparks in the laser focus. At both the shorter and the longer wavelength end of the spectra, the emissions measured are obviously intense than calculated one. For the shorter wavelength, the continuum is emitted from highly ionized stages generated in the center of plasma by the laser intensity more than $3.5 \times 10^{12}$ W/cm². On the other side, the continuum at the longer wavelength is contributed by the lowly ionized particles in the plasma of low density. The synthetic spectrum from the CR model code is good enough to reproduce what had taken in the laboratory. Figure 2 shows the charge state fraction of the ionization stage which is averaged during the laser pulse interaction, where the electron density located at the range between $5 \times 10^{19}$ cm⁻³ and $5 \times 10^{20}$ cm⁻³, the electron temperature is above 100 eV in the simulation. Since the measured soft x-ray emission is mostly from the high density and high temperature plasma part in the experiments, the calculation is comparable to that in the experiments. The molybdenum atomic level population distributions extracted from the measured spectra can be used as the pre-plasma analysis for the Nickel-like molybdenum soft x-ray lasers.

4. Conclusion
A Collisinal-Radiative model code with fine atomic data included in the hydrodynamic code was developed. A good recombination continuum shape agreement between the simulation and the semi-empirical calibrated Mo plasma experiment spectrum was obtained over the whole wavelength scale. The intensity mismatch at both wings of the two spectra was attributed to the intensity distribution of the laser focus, which is a Gaussian one in experiments, and a flat-top one assumed in the numerical calculations. With such a time dependent CR model code, plasmas information can be extracted from the measured spectra directly.

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