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A detailed collisional radiative model for Ti plasma

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Titanium plasmas are widely studied due to their applications in thin-film deposition, biomedical coatings, and advanced material processing. Accurate plasma diagnostics are essential for optimizing these applications, with laser-induced breakdown spectroscopy serving as a powerful non-intrusive technique. A reliable collisional radiative (CR) model is crucial for extracting plasma parameters such as electron temperature and electron density from spectral emissions. However, existing Ti plasma studies are limited by the lack of comprehensive atomic and collisional data. This study presents a detailed CR model for Ti plasma by validating it using laser-induced breakdown spectroscopy (LIBS) measurements of Mejia et al. [1]. Radiative rates for 194 fine-structure levels considered in the model of Ti I are computed using the multiconfiguration Dirac-Hartree-Fock (MCDHF) method. Electron impact excitation cross-sections are calculated from the ground and metastable sates $3d^2 4s^2$ (a ^3F , a ^1D, a ^3P) and $3d^3 4s$ (a ^5F) up to upper fine structure levels using relativistic distorted wave (RDW) [2] theory for a wide range of incident electron energy from excitation threshold to 250 eV. The CR model incorporates key plasma processes, including radiative decay, electron impact excitation, and de-excitation, ionization, and three-body recombination. Incorporating all of the key plasma processes into a collisional radiative solver, a system of rate equations is solved to get the upper-level population of the fine structure energy levels. Theoretical spectra are generated and compared with experimental LIBS measurements from Mejia et al. [1] for validation. Eight Ti I spectral lines are analyzed and electron temperature (T_e) and density (n_e) at different delay times of 0.5 and 3.5 μs are extracted. A strong agreement between computed and experimental results confirms the accuracy of our model. The validated atomic data and CR model pave the way for future applications in Ti plasma studies.

The intensity of an emission line ($f \rightarrow i$) I_{fi} related by the following relation with the upper-level population (n_f), radiative decay rate (A_{fi}) and the electronic transition energy (E_{fi}) as,

$$I_{fi}\ \alpha\ n_f\ A_{fi}\ E_{fi}$$

The theoretical and experimental intensities are normalized by the following equation,

$$I^N_{k,CR(exp)} = \frac{I_{k,CR(exp)}}{\sum_{k=1}^{8} I_{k,CR(exp)}}$$

We have to find the T_e and n_e for which the deviation parameter defined by the normalized CR model and experimental intensities as,

$$\delta = \sum_{k=1}^{8}(I^N_{k,CR} - I^N_{k,exp})$$

will be a minimum. Figure 1 shows the comparison of theoretical and experimental intensities at 3.5 μs delay time for the optimized $T_e = 0.76$ eV and $n_e = 5.0 \times 10^{17}$ cm^{-3}. The detailed results will be discussed in the conference.

References
[1] R. E. Mejia, M. Raineri, R. Sarmiento, J. C. A´lvarez, P. Pacheco, Laser Plasma Characterization and Atomic Structure Calculations of Ti II, IEEE Transactions on Plasma Science 51 (10) (2023) 3035–3052.
[2] L. Sharma, A. Surzhykov, R. Srivastava, S. Fritzsche, Electron-impact excitation of singly charged metal ions, Physical Review A 83 (6) (2011) 062701.

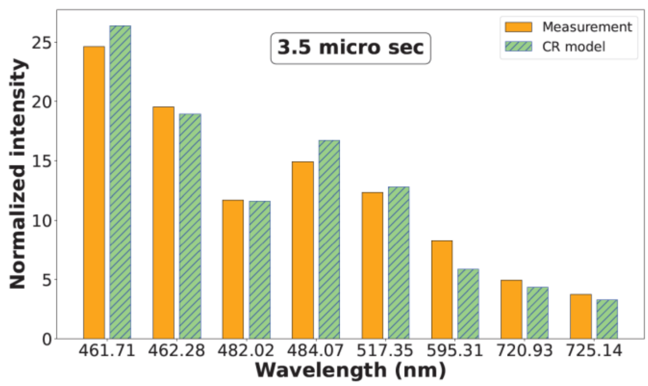

Figure 1: Comparison of normalized intensity from the CR model and experimental measurements for optimized T_e and n_e at plasma delay time 3.5 μs.