P39

Fully relativistic calculation of cross sections and their application in identifying suitable emission lines for the diagnostics of non-equilibrium plasmas

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Accurate plasma diagnostics are essential for comprehending their physics and practical applications in various fields, including astrophysics, fusion research, semiconductor manufacturing, and so on. Spectroscopy-based diagnostic techniques serve as potent tools for characterizing various types of plasmas, including those found in extreme conditions such as fusion plasmas. Optical emission spectroscopy (OES) is the commonly employed spectroscopic technique due to its non-invasive nature and robustness. Yet, achieving accurate characterization necessitates the integration of OES measurements with appropriate plasma population kinetic models. However, it's important to note that most of the plasmas we deal with deviates significantly from complete/local thermodynamic equilibrium and hence the equilibrium models are no longer applicable. Collisional Radiative (CR) model is a prominent population kinetic model extensively utilized for the diagnostics of non-equilibrium plasmas. It helps in extracting plasma parameters, tracking their spatio-temporal evolution, and in identifying emission lines suitable to probe the qualitative behaviour of plasma parameters in real-time monitoring. The mechanisms that populate and depopulate the emitting states constitute a coupling between the collisional and radiative processes inside the plasma. The excitation mechanisms that result in plasma emission are dominated by the inelastic collision of plasma electrons with atoms, molecules, and ions. Hence, it is crucial to calculate the cross sections for electron impact excitation processes accurately.

In light of this we have performed the calculations of fine structure resolved excitation cross sections using the relativistic distorted wave approximation theory with the aid of multi configurational Dirac Fock wavefunctions as the target states *i.e.,* Mo, Sn, Ga and Al, for a wide range of incident electron energies (threshold to 500 eV) [1, 2]. The accuracy of the wavefunctions employed in our calculations is validated by comparing excitation energies, oscillator strengths, and transition probabilities with previously reported results. The calculated cross sections are compared with available measurements and calculations to ensure their consistency. Furthermore, the calculated cross sections are successfully implemented in the CR model for the diagnostics of various non-equilibrium plasmas of Mo, Sn, Ga and Al [1, 2]. In addition to this, suitable line ratios for the determination of the plasma parameters are also proposed. The detailed results, along with methodology and discussions, will be presented at the school.

[1] Indhu Suresh et al, Plasma Sources Sci. Technol. **32**, 075006 (2023).
[2] Indhu Suresh et al, Plasma Sources Sci. Technol. **31,** 095016 (2022).