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# Tungsten Collisional-Radiative Models in support of impurity-influx measurements

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## *State of the art and motivations*

Material choice for the plasma facing components in fusion experiments is determined by competing desirables: on the one hand the material should have a high thermal conductivity, high threshold for melting and sputtering, and low erosion rate under plasma contact, and on the other hand as a plasma impurity it should not cause excessive radiative energy loss.

For the ITER tokamak, currently under construction at Cadarache, France [1], Tungsten (symbol W, atomic number 74) is the favoured material for the wall regions of highest particle and heat load in a fusion reactor vessel, with beryllium for regions of lower heat and particle load. ITER is to start operation with a W-Be or W wall for the main D-D and D-T experimental programme. In support of ITER and looking ahead to the prospect of a fusion reactor, other experimental plasma groups are also considering tungsten, including the ASDEX-Upgrade tokamak which now operates with an all-W wall and at JET (Joint European Torus) facility in Oxford. Smaller-scale experiments involving tungsten tiles are carried out on other tokamaks. Researchers from the CTAMOP group have an ongoing relationship with magnetically-confined experimental groups at JET and both Auburn University and D-III-D, General Atomics in the US. *One of the major questions that these experimental groups are addressing is the determination the impurity influx from plasma facing components under ITER conditions.*

Atomic processes are central to energy transfer in magnetically confined plasmas. The energy balance in fusion devices such as tokamaks depends critically on how the plasma interacts with the walls of the vessel, demanding accurate cross sections and associated rates for a wide variety of collisional processes. At Queens, we develop both the theoretical methods and computer codes to provide accurate predictions of the atomic structure, electron-impact excitation/ionization and recombination rates that underpin the interpretation of these observations [2].

These rates will enable us to understand and mitigate the causes of critical radiation losses that in minuscule concentrations prevent ignition. For modelling the behaviour of tungsten in a plasma a comprehensive understanding of most collisional processes is required for many ion stages. Beyond the first few charge states of Tungsten, open 4d and 4f shell configurations require complicated atomic structure calculations, and equally demanding electron-impact collisional calculations [3].

## Objectives & Methodology

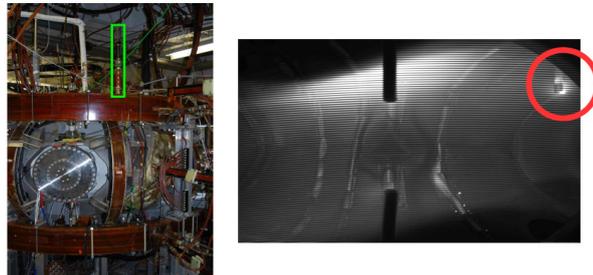
The project shall proceed as follows. There shall be a review of the underlying electron-impact driven collisional processes as well as collisional-radiative theory. The student will familiarize themselves with the numerical procedures required to provide rates, as well as solving the rate equations for a variety of distributions, starting initially with the Maxwellian. If any of the collisional processes are missing from the rate equations, we shall calculate them. One of the key theoretical methods, R-matrix theory has been pioneered at Queen's and shall be employed for the majority of the collisional rates. A large aspect of the project, shall be the interaction with experimental groups that carry out impurity measurements. Therefore, if they determine that a particular spectral line is important, we shall tailor our theoretical calculations to optimize the atomic structure and collisional calculations for that line.

Specific objectives of the projects are:

- To provide the student with a complete survey of the collisional processes involved with plasma collisional-radiative modelling. To take first principle atomic calculations through to a valuable application.
- There is a strong computational aspect, therefore an interest in computational modelling, and in particular utilizing powerful parallel supercomputers is required.
- There will be a strong collaboration between experimental groups in the US and researchers at Queens. Identifying strong spectral lines observed from various experimental devices under particular temperature and density conditions shall be an integral part of the project. However, theoretically, collisional radiative modelling should allow us to be more proactive in suggesting diagnostic lines for the experimental groups to observe.
- The Phd student shall have to respond to experimental requests in quite short timeframes, due to the cyclical nature of experimental measurements on large scale devices.
- To acquire good programming and numerical skills valuable for graduate level work, which are also marketable skills within the workplace.

This project shall bring together the efforts of the CTAMOP group at Queen's, the theoretical group at Auburn University as well as experimentalists working on the Compact Toroidal Hybrid experiment, also at Auburn University. We shall also collaborate with plasma experimentalists at the D-III-D facility, General Atomics, CA, USA.

## Required skills



**Fig. 1:** The left-hand figure shows the Compact Toroidal Hybrid (CTH) experiment at Auburn University. The green rectangle highlights the port from which a small metal cube of tungsten is injected into the device. The right-hand figure shows the emission of infra-red lines from this cube from within CTH under normal operating conditions.

It would be beneficial if the prospective student has had an entry-level quantum mechanical course. There is the intent that the student would develop, with guidance, their own collisional-radiative model. Therefore, some basic understanding of numerical methods with either Matlab, C++ , Fortran or their more modern equivalents would be desirable. However, more important is an interest in the topic as these skill-sets can be acquired during the project.

#### Further information

For further information, please contact the project supervisors Dr. Ballance and/or Dr. Ramsbottom: [C.Ballance@qub.ac.uk](mailto:C.Ballance@qub.ac.uk) and/or [c.ramsbottom@qub.ac.uk](mailto:c.ramsbottom@qub.ac.uk).

## References

- [1] <http://www.iter.org/>
- [2] R-Matrix Theory of Atomic Collisions, Springer, ISBN-10: 3642159303 (2011).
- [3] C. P. Ballance, S. D. Loch, M. S. Pindzola, and D. C. Griffin, *J. Phys. B: At. Mol. Opt. Phys.* **46**, 055202 (2013).