Beam-plasma atomic data needs for fusion devices

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Modelling of the attenuation of heating and diagnostic H/D/T beams in fusion plasmas is important for calculating the transmission of beam power through the plasma and the potential for damaging heat loads on machine structures. Uncertainties in attenuation of the ITER diagnostic beam by the time it reaches the centre of the plasma are acknowledged in the design of the charge-exchange diagnostic which will measure both beam emission (as a diagnostic of the local neutral beam density as well as impurity charge exchange. However, the calculated beam transmission affects the anticipated signal levels in the centre of the plasma and hence the signal-to-noise performance projected for the diagnostic. Good cross-section data for the impurity charge-exchange and beam emission processes are required for the quantitative analysis of these spectra. (Lineshape analysis—Doppler shift and broadening—is potentially affected by the fine structure of the impurity emission lines but these effects are insignificant at the temperatures of interest.)

Simulations of the D-alpha spectrum from tokamaks (developed to study the emission spectrum due to charge-exchange between fast deuterons and D heating beams—Fast Ion D-alpha—FIDA) need to accurately model the spectrum due to all processes. Among these is charge-exchange between D+ and D0 at the plasma edge for which state resolved cross-sections are needed.

The Motional Stark effect (beam emission) is applied on many Tokamaks with polarisation measurements used to measure the local magnetic field directions. Alternative measurements that use the intensity ratios of the sigma and pi lines depend on there being a given ratio of the populations of the upper states, any perturbation from statistical population would affect the interpretation.

Neutral lithium beams with energies of order 60keV are used in many fusion experiments to measure the edge electron density profile through the rate of attenuation of the beam. In fusion experiments with a lithium coated first wall the intrinsic lithium emission from the plasma can blind the beam diagnostic. In these cases the use of sodium neutral beams is being explored. Thermal energy helium gas jets are used in some experiments as a simpler alternative to the lithium/sodium. The rate processes for beam attenuation, excitation and charge-exchange for these injected neutrals are needed for the quantitative interpretation of the emission spectra.

Reionisation of heating beam neutrals can occur due to collisions with neutral gas in the ducts of the beam systems. At high neutral pressures this can lead to sufficient density of ionised particles as to pose a risk to machine components when the particles enter the plasma confining fields. Atomic data would be needed to model this process.

Atomic Data for CXRS and BES/Stark Diagnostics

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Several projects carried out recently were described illustrating the large scale calculation of data relevant to neutral beam heating/diagnostics in fusion experiments. For example, work to produce state-selective charge transfer data for CXRS involving Ar were described. First treated comprehensively in the 1990’s [1] data were computed for Ar^{2+} + H(1s), tabulating the n- and nl-resolved charge transfer cross sections for several energies relevant to neutral beam diagnostics at the time. The data were disseminated via the website of the ORNL Controlled Fusion Atomic data Center [2]. With an eye to ITER relevant neutral beam energies, this database was extended about ten years later to include higher impact energies, and also excited state H targets (H(2s), H(2p)) [3,4].

The method used to compute these data (again, recalculated for the relevant beam energies) was stringently tested by spectroscopic experiments at TEXTOR [5] confirming the results, and thus showing their utility for interpretation of CXRS measurements at present devices and for ITER. Similar work was also shown regarding the feasibility of CXRS for ITER using W^{64+} [6]. In this work, it was found that a number of strong lines arising from charge transfer with a neutral hydrogen beam
in the VUV visible spectral range should be available for diagnosis of the likely most abundant tungsten ion in ITER core plasma. The results were obtained using newly calculated state-selective charge transfer cross sections and a detailed collisional-radiative model including thousands of levels populated by either electron-impact or charge transfer with the neutral beam.

Finally, relevant to beam emission spectroscopy and motional Stark effect spectroscopy, data and collisional-radiative modeling were reviewed that recently showed that the typical statistical assumptions about state distributions in plasma are not valid [7], point the way toward more complete ability to utilize neutral hydrogen beam excitation in diagnostics. Data for that work [8], consisting of full density matrix elements for H⁺ exciting H(1s) to levels within n=2,3, and 4, from a few hundred eV to 2 MeV collision energies, provided during work of a previous IAEA CRP.


Charge-transfer collisions involving few-electron systems
T. Kirchner

Ion-atom collision systems that involve more than one electron constitute nonseparable few-body problems, whose full solution is difficult to say the least. At impact energies well below 1 keV/amu an expansion of the stationary scattering wave function in terms of a limited number of products of nuclear and molecular state wave functions (amended to satisfy scattering boundary conditions) is feasible and usually sufficient to obtain accurate charge-transfer cross sections provided the electronic wave functions include configuration interaction (e.g. [1]).

At energies above 1 keV/amu this approach becomes inefficient and close-coupling methods within the semi classical approximation are better suited to treat the problem. For bare-ion collisions from helium target atoms explicit solutions of the two-electron time-dependent Schrödinger equation can be achieved, but are computationally costly and cannot be extended to problems which involve more than two electrons.

Approximate alternatives are thus necessary to deal with more general situations. The independent electron model (IEM) represents a convenient and often quite accurate framework to carry out charge-transfer calculations for many-electron collision systems. We have used the IEM, e.g., to calculate (n,l)-specific cross sections for single capture in Ne²⁺ impact collisions with He, Ne, and Ar atoms. One motivation for this work has been the availability of experimental data for Lyman α and Lyman β⁺ emissions after shell-specific single capture. When coupled with radiative cascade calculations our IEM results show good overall agreement with the measurements [2].

Time-dependent density functional theory provides a firm footing of the IEM and gives some hints of how to improve the calculations. In this context, we have investigated the use of correlation integrals in the final-state analysis of one- and two-electron processes in proton and He²⁺- He collisions [3]. Particularly for the case of double capture, for which the IEM has the tendency to overestimate the cross section, this has improved the agreement with experimental data.