Atomic Data For Core And Edge Modeling

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Abstract. Future magnetic fusion energy devices, will have both very high Z (tungsten) and low Z (beryllium) plasma facing components, are setting the agenda for current atomic data needs. Data for the light species are in good shape but the heavy species present some challenges. We outline an approach for systematic heavy element data production for fusion applications in addition to techniques for handling the large amount of data in modeling codes efficiently.

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INTRODUCTION

The challenge presented by ITER to atomic physics almost demands two different worldviews of data provision. Data for modeling the combination of very high and very low Z plasma facing components means that a single approach is not feasible.

Tungsten, with its 74 ionization stages, will stress the computational size and running time of 2-D and 3-D cell-based plasma models. Even if the increase in turn-around speed was acceptable, given that computers improve year on year, numerical instabilities arising from manipulating very small rate coefficients, are a great concern. On the low Z side, well established collisional-radiative models with very many n-shell methods to account for step-wise ionization and dielectronic recombination [1] properly describe the effective coefficients required for finite density modeling.

The variation with temperature in coronal equilibrium balance, at a fixed density, for metastable resolved beryllium and stage resolved tungsten shown in figure 1 illustrates the scale of different requirements. The simple atomic structure of all Be ions results in a spectral emission composed of isolated lines. For tungsten this simplicity is found only in the very highly ionized stages, which require temperatures of 25–30keV to produce, outside the capabilities of present day magnetic fusion energy (MFE) devices and are unlikely to be seen in ITER. Their complex atomic structure (partially filled $d$ and $f$ shells) give rise to broad emission features punctuated with some strong lines [2].

Fundamental cross sections for excitation, ionization, recombination and charge exchange, along with atomic structure, must be mediated through population models to provide the effective source rates, line and spectral feature emissivities and power coefficients for MFE models, diagnostic interpretation and predictive models. These are termed derived data.

For light elements the quality of the fundamental data is high. For the rest it is
FIGURE 1. Ionization balance in coronal equilibrium for beryllium in the metastable resolved form and tungsten in the stage-to-stage representation. The density is fixed at $10^{19} \text{m}^{-3}$ and the temperature range is representative of the range of tokamak condition from the edge/divertor to the core.

not feasible, or perhaps even desirable, to calculate all the fundamental reactions at the highest precision. However comprehensive coverage is still required for plasma modeling. Our approach is a layered one. Coverage is provided by baseline quality calculations. This sets up the structure into which can be embedded high quality work which is targeted on those ions which are important for either diagnostic or ionization state dynamics.

As import is the efficient handling of the derived data efficiently in MFE plasma codes. For heavy species we have developed strategies based on grouping similar stages, called *superstages*, to reduce the quantity of data without a significant degradation in the plasma model predictions. For the lighter elements, and some stages in heavier elements, the use of a fully metastable resolved picture for tracking the ionization stage evolution may be more appropriate. Both resolution can co-exist in the iso-nuclear data.

The practical realization of these approaches to data production and handling are incorporated in ADAS [3].

**SYSTEMATIC HEAVY ELEMENT DATA GENERATION**

The urgent questions to be answered for ITER cannot wait for the slow delivery of light element quality data, such as state selective excitation, dielectronic recombination, ionization and charge exchange, one iso-electronic sequence at a time. The delivery must be accelerated. We identify three levels of resolution: configuration average (*ca*), Russel-Saunders (*ls*) and intermediate coupling (*ic*) which leads to a baseline set of data.

For spectral and power data the Cowan code [4] has been used to calculate the atomic structure and the effective collision strengths in the Born approximation: the accuracy of using Born is addressed later.

There are 180 different ground configurations for ions of all elements up to radon.
The non-hydrogenic filling order accounts for the changing ground state along an iso-electronic sequence. We require a set of excited configurations for the structure and population models of the baseline data collection and for systematic data production a rule based promotion strategy is used to automate the selection. The rule-chosen set can be supplemented with or reduced by user supplied configurations if desired. As an example consider $W^{+20}$ with a 4d$^{10}$4f$^7$ ground configuration. One rule is to promote one of the valance 4f electrons to 5\(\ell\), another to promote one of the closed 4d shell electrons to 4f and 5\(\ell\) and, given that they lie below the ionization limit, the 4p electrons can also be promoted. Other rules such as the \(\Delta n\) of valence shell jumps, filling of a complex, restrictions on depth of inner shell promotions etc. may be relevant for different ions. Figure 2 shows the rising number of levels as the promotion rules admit more and more configurations.

![Figure 2](image)

**FIGURE 2.** For $W^{+20}$ the number of levels rises as the promotion rules are amended. The dotted line indicates where a reasonably large $ic$ or $ls$ coupled calculation would have stopped. The difference in radiated power between this stopping point and by including all configurations is a factor of 2.

The structure calculation must be sized to available computer resources. This gives rise to the danger that the (necessarily) limited set of configurations does not capture all possible pathways. The omitted configurations will be manifested by missing spectral emission and an underestimation of the radiated power. An adjunct calculation in the computationally more tractable $ca$ resolution, which can include many more configurations, will indicate whether the emission of any omitted configurations lies within the spectrum of interest. For confrontation with measured spectra or instrument design studies it is best to re-run the structure calculations to include them, perhaps at the expense of omitting others.

The $ca$ calculation is also the way to account for the underestimated power. The total power is the summed power from all transitions generated in a collisional-radiative model. However there can be differences in the total power between the three resolutions, particularly if open 4d and 4f shells are involved. The energy of the ground configuration in $ca$ resolution is a mean of the wide distribution of energies possible in the $ic$ picture and consequently will over-estimate the power. For more excited configurations the discrepancy diminishes and, as there is no real computational limit to the number
of \(ca\) configurations, the difference in radiated power between a large set and a set corresponding to the \(ic\) configurations can be added as top-up power to the \(ic\) calculation. Figure 3 shows the power gap for various elements as different shells open up.

**FIGURE 3.** The power ‘gap’ for various elements as the shells open up, evaluated at an electron temperature corresponding to the ionization potential and density of \(10^{19} \text{m}^{-3}\). The gap is the top-up power required for the total power coefficients.

With increasing atomic number relativistic effects increase in importance. Ni-like xenon, \(\text{Xe}^{+26}\), with a \(3d^{10}\) ground configuration, is on a shell boundary and has one active electron in the excited state. The effect of substituting a Dirac R-matrix calculation for this stage [5] into a baseline quality dataset is shown in figure 4. The Born results give a reasonable qualitative description of the spectral signature. However, quantitatively, the R-matrix based emissivities differ by a factor of two for the 3d–4p feature, while

![Composite Xe^{26+} : Baseline Xe^{26+} : DARC](image)

**FIGURE 4.** Spectral emission in the 10–12Å region. The emission is assembled from the baseline feature photon emissivity coefficients of each ionization stage and combined with the ionization balance at an electron temperature of 500eV and density \(10^9 \text{m}^{-3}\). The emission of the \(\text{Xe}^{+26}\) stage is shown in red. The effect of including the feature photon emissivity coefficient from the GRASP/DARC calculation is shown in blue.
the dominant 3d–4f feature is about two thirds smaller than the Born, changes directly attributed to the differences in the collision strengths. Interpreting the difference as an uncertainty range suggests that using Born collision strengths is well suited for systematic data production at baseline quality. The importance of improving key stages is seen in recent calculations for the analogous stage in tungsten, W^{+46}, and the adjacent W^{+45} and W^{+44} stages [6], where radiation damping is shown to be important for some transitions.

Comparisons with EBIT spectra [7] show acceptable agreement for wavelength predictions.

Ionization balance enters the state equation in plasma models as source (ionization) and sink (recombination) terms. Universal coverage for heavy species has relied on simple parametric forms to evaluate these rate coefficients [8].

For ionization one of the most used is the Lotz formula [9], requiring only oscillator strengths, ionization potentials and excitation energies, but which is limited to direct shell contributions to the total rate. For realistic rates for heavy species excitation-autoionization (EA) effects cannot be neglected. Nevertheless for quick estimates of unfamiliar species, this method is still in use and provides an adequate source of data. For heavy species the most powerful theoretical methods are likely to be applied to very few stages. However for baseline data an increase in quality, to account for missing EA, is desirable. The method adopted in ADAS is configuration average distorted wave (CADW) [10] which calculates shell direct cross sections, Auger breakup and the competing radiation damping. All data in the tungsten iso-nuclear set have been calculated [11] and are compared to simple parametric forms in figure 5, which shows the lift in quality. The CADW method is amenable to systematic data production and the sets of configurations can be generated from a number of compact promotion rules.

For fusion plasma conditions recombination can be separated into radiative and dielectronic parts, the independent process approximation. A high atomic number or charge does not affect calculation of the radiative part following [13]. On the other hand, state selective dielectronic recombination calculations can become overwhelming. A hierarchy of calculation methods of increasing sophistication, described in [14] as part
of a comprehensive co-ordinated effort to generate dielectronic data for fusion and astrophysics, outlined the Burgess-Bethe general program (BBGP) method suited to data production for heavy species ions.

**SUPERSTAGES FOR HEAVY ELEMENT MANIPULATION**

Atomic physics underpins many of the core and edge modeling codes and estimates of the performance of, eg. the divertor and radiating mantle, will rely of accurate atomic data. Adding tungsten to these codes is not just an incremental step-up from carbon.

The timely production and improvement in quality for heavy species is the first step. Handling the quantity of the resulting data in the models is just as important. An element in a plasma is described by the abundances of all metastables of each ionization stage, which are linked to each other by ionization and recombination coefficients\(^1\), whose populations evolve on similar timescales as transport. The spectral features and power coefficients are quasi-static with respect to and are driven by these evolving populations.

Typically edge codes divide the plasma into a mesh of cells, counted in the thousands to millions depending on the granularity of the transport phenomenon under investigation. The ionization state of each impurity in the cell must be stored, which for tungsten is 75 stages many of which will be near zero. Re-calculating the balance at each time step may be subject to numerical instabilities when manipulating the very small rates of ions far from their temperature of maximum abundance.

In a fusion plasma groups of neighboring stages in mid to high-Z elements act in a similar way. A measure of this is the change in fractional ionization potential with Z; it is relatively unchanging but is punctuated with sharp peaks when the shells open. The peaks in figure 6 suggest a natural way to partition an element into the influential and less distinguishable stages, both from a diagnostic and ionization balance point of view.

Ionization stages at and adjacent to the peaks remain as individual stages but those in between are grouped into a superstage. Within the superstage the distribution is given by coronal equilibrium. Note that the neutral stage should not be part of a bundle since it reacts differently to the magnetic field. For tungsten the natural partition reduces to 35 superstages but more targeted partitions are used for edge modeling where the terminal charge state may be low depending on the maximum temperature in the model. Figure 7 shows that the superstage approach works well for core simulations and even with very aggressive bundling descriptions is robust in describing impurity behavior in the scrape-off-layer (SOL) \([15]\). The superstage approach can mix multiple resolution levels in one dataset — plasma conditions, such as steep gradients, may be best described by following metastables but superstage to superstage may be more appropriate elsewhere in the model.

The changes required of existing plasma codes are modest. The indexing is no longer represented by the ionization stage. For calculating electron energy loss or neo-classical coefficients, \(Z, Z^2\) and the energy difference between the superstages are now functions of temperature and density necessitating the introduction of three new coefficients.

\(^1\) And cross coupling coefficients for metastables within a stage.
FIGURE 6. (left) ‘Natural’ partition of tungsten defined by a variation ($\sigma = 1.5$) around a running mean. (right) Different asymptotic behavior of the recombination coefficient between stage to stage and superstage to superstage cases.

FIGURE 7. (left) Comparison of increasingly aggressive bundling schemes for core tungsten — impurity content, radiation and electron cooling loss. (right) Tungsten density along the separatrix for two 9-member superstages. the red curve has more aggressive bundling at the lower stages.

**ATOMIC DATA FOR LIGHT ELEMENTS**

For present day machines the focus has been on the light elements; beryllium, carbon and boron for first wall materials, nitrogen and neon for control along with the fuel species and helium have all received scrutiny. The most recent assessments for lithium [16] and beryllium [17] show the importance of using the most sophisticated codes for the neutral and near neutral species. Reworking of selected stages of boron, carbon and oxygen is underway. Generalized collisional-radiative (GCR) modeling properly describes the behavior of light ions in the metastable resolved picture. This was strikingly confirmed
by lithium observations on DIII-D [18] where the both the new data revision and
the density dependence of the effective coefficients were required to fully explain the
experimental measurement. The GCR review [1] described the theoretical background
and assessed the quality of fundamental data required to generate the derived GCR
coefficients.

More work on fundamental data is needed. Improved excitation data for neutral neon,
where coupling to the target continuum can have large effects on the electron-impact
excitation cross sections, is required but work is underway to address this. Fluorine has
been missed out but, as a constituent of teflon, may be important and should be updated.
Argon is an important element because of its importance for active radiation control in
ITER. The difficult lowly ionized stages have been considered already [19, 20].

Although not a light element one of the unaddressed problems is that of neutral
tungsten. It shares the difficulty in calculation of the light neutrals but its atomic structure
is more difficult having many more levels. Direct observation of the influx sources is
valuable for estimating the impurity influx. In a tokamak environment the most suitable
line to measure, $^7\text{S} - ^5\text{P}$ at 4009Å is metastable. Empirical methods are used to assemble
an ionization per photon coefficient ($S/XB$: ratio of ionization rate to excitation rate
times branching ratio of a transition) [21] in order to relate photon to particle fluxes.

SUMMARY

The availability of fundamental atomic data in expectation of ITER is in a good state
for the light elements, but less so for heavy species. A strategy for providing universal
coverage, or an improved baseline, has been outlined. Methods for the economical
handling of the large quantities of data flow naturally from a consistent multi-resolution
partitioning of an element. Here metastable resolved, stage to stage and superstage
resolutions, grouped according to model or diagnostic requirements can coexist in the
datasets used by modeling codes. Challenges remain, notably for the for the neutral and
near-neutral high-Z stages, but the light element neutrals were in a analogous state just
a few years ago.

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