# **Atomic Data for Tungsten in Fusion Devices**

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In future fusion devices tungsten will play an important role as first wall material [1]. However, when using tungsten in a reactor, the central tungsten concentrations must be below  $10^{-4}$  to avoid unduly large radiation losses [2]. This delicate situation calls for a dedicated development of diagnostics tuned for tungsten. An integral part of this effort is the availability and improvement of atomic data. New extensions of ADAS [3] have been employed to provide a consistent set of data for all ion states of interest. Using the Cowan-code [4], the necessary electron collision cross sections are obtained. In this paper, first results of these calculations will be compared to measurements of tungsten spectra and radiated power that have been taken at ASDEX Upgrade.

#### **Atomic Data from the Cowan Code**

The complex electron structure of high-Z elements is the main reason for the absence of atomic data covering ionisation-recombination coefficients, spectral emission data and corresponding cooling factors. Low quality coarse data is available from the average ion model (AIM) [6], but in this model no spectral distribution of radiation is possible. At the other extreme computational limits make high quality R-matrix calculations suitable only for special ion states with a sufficiently simple electron structure. There are data for several ion states from the distorted wave (DW) code HULLAC [5], however, the data are not available in a general context with ionisation and recombination data and cooling factor. The new ADAS extension sets up an infrastructure for all ions with intermediate quality data calculated with the Cowan code [4]. Future upgrades of selected ion states with high quality data are easily possible due to the modular structure in ADAS. The Cowan code calculates collisional data using the plane-wave Born approximation (PWB), which treats the incoming and outgoing electrons as plane waves. This simplification is good (cross sections errors < 50%) for energies larger than 3-4 times the ion potential. Below these values the accuracy of the cross sections decrease. When considering a plasma with a Maxwellian electron distribution the low energy discrepancies for cross sections show up less pronounced in the corresponding rates. Care must be taken in the interpretation of individual spectral lines as the PWB atomic data will give larger uncertainties than the higher quality methods (R-matrix, DW). However, the PWB data is very suited to interpreting the radiated power of line arrays. For these, the errors of the individual spectral lines statistically tend to cancel. The calculated excitation rate coefficients, A-values and energy levels are the inputs to a collisional-radiative model where level populations are derived for different plasma parameters. Subsequently, data for bulk radiation, radiation in certain wavelength regions and spectral emissions are calculated.

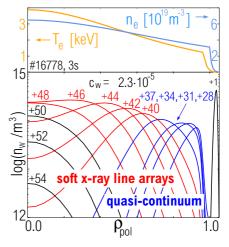
## **Experimental Set-Up**

ASDEX Upgrade has been operating successfully with tungsten coated plasma facing components in the campains 2002/2003 with  $14.6\,\mathrm{m}^2~(\hat{=}35\,\%)$  and  $24.6\,\mathrm{m}^2~(\hat{=}65\,\%)$  in 2003/2004 [7]. Additional impurities (Hf, Ta, Re, Au, Pb, Bi) could be injected quasi-continuously with 20Hz by the laser blow-off (LBO) system. Various spectrometer and bulk radiation diagnostics cover the wavelength region  $0.1-100\,\mathrm{nm}$ . In this paper spectra of tungsten in the region

0.4 nm - 0.8 nm and at 5 nm are presented. The first wavelength region is covered by a Bragg scanning crystal spectrometer that recorded the spectra with an ADP crystal (2d = 1.064 nm) using a Multi Strip Gaseous Chamber. The wavelength accuracy is better than  $10^{-3}$ . An error of 50% is attributed to the absolute values. The spectra at 5 nm are obtained via a Grazing Incidence spectrometer with detection via a microchannel plate and a phosphor screen captured by a CCD camera; the wavelength uncertainty is in the range  $\sim 2 \cdot 10^{-3}$ . The absolute photon fluxes are only estimates (within factor 5), as the calibration was obtained indirectly by modelling of H- and He-like spectral lines of boron, based on charge exchange concentration measurements. Both spectrometers' lines of sight (LOS) are close to the midplane and cross the plasma close to the horizontal in the poloidal plane which ensures measurements include emission from the center of the plasma. The excact geometry is considered in the modelling and special attention is devoted to the self-consistency between the spectral emissivity and the total radiation. A bolometer with many LOS is used to measure the total radiation with a tomographic algorithm applied to determine the total radiated power along the plasma radius. Diagnosing the radiated power due to tungsten requires that special calibration discharges are performed at the beginning of each campain. The spectral line of Ni-like tungsten at 0.793 nm and the emissions of the tungsten quasicontinuum at 5 nm are related to the increase of total radiation due to a tungsten LBO. The total radiated power emitted by tungsten is then determined in any following discharge by diagnosing the tungsten emissions and interpreting them with the actual plasma parameters.

## **Analysis/Discussion**

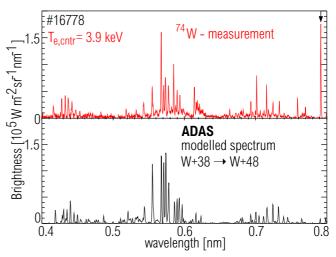
The modelling of spectra needs to take into account the abundance of each contributing ion state along the LOS of a spectrometer. In [8] transport was found to have small effect on the ionisation balance. Nevertheless, its influence was taken into account using STRAHL with the assumption of typical diffusion coefficients and such drift velocities that a constant tungsten concentration within  $\rho_{pol}=0.95$  is obtained. Ionisation and recombination data, which are about to be supplied by ADAS, are here taken from [8], i.e. modified ADPAK [6] data. Fig. 1 shows the distribution of tungsten ion states for the discharge #16778 in which the tungsten spectrum, shown in fig. 2, has been measured. The upper part of fig. 2 shows the spectral region in the



**Fig.1:** Tungsten ion densities vs. plasma radius for  $c_W = 2.3 \cdot 10^{-5}$ 

soft X-ray (SXR) range, which contains more than 90% of the detectable emissions of tungsten below 2 nm, in this discharge. This is compared to a modelled spectrum using the new excitation cross sections from ADAS. The wavelengths of modelled spectral lines show small deviations. As expected, there are differences in the intensity envelope between the measured and modelled spectrum but the basic structure of the emissions, i.e. the coarse distribution of emissions in the spectrum is well reproduced. A particularly large deviation (factor  $\approx 15$ ) is observed for the electric quadrupole line at 0.793 nm (3d<sup>10</sup> J=0  $\rightarrow$  3d<sup>9</sup>4s<sup>1</sup> J=2). Comparison of the direct cross sections and A-values from HUL-LAC [5] for this special transition show agreement to the corresponding ADAS values, however, the HULLAC data underestimates this spectral line only by a factor of 2 [9].

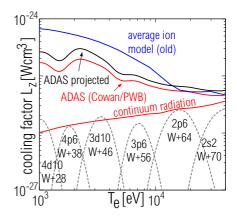
The missing fueling of the upper level for ADAS must be analysed by looking at the details of the collisional-radiative modelling. It was pointed out by [5] that about 30% of the upper level population for HULLAC originates from inner shell ionisation of W<sup>+45</sup> (3d<sup>10</sup>4s<sup>1</sup>) a process that is not yet considered in ADAS. Further investigations are going on. For the modelling of the spectrum in fig. 2 the assumed tungsten concentration  $c_W$  was scaled such that the modelled and measured spectra show the same integrated emissivity. This lead to the conclusion that  $c_{W,spec} = 2 \pm 1 \cdot 10^{-4}$ . Alternatively,



**Fig.2:** Comparison of measured tungsten emissions and the corresponding modelled spectrum.

 $c_{WADAS} = 2.0 \pm 0.5 \cdot 10^{-4}$  was derived from the total radiation, interpreted with a cooling factor based on ADAS data. Evaluating the total radiation with data from the AIM results in  $c_{W,AIM} = 8 \pm 2 \cdot 10^{-5}$ . The given uncertainties are purely experimental. The spectrometer and total radiation measurement are consistent when both are interpreted with atomic data from ADAS. When interpreting the total radiation with the two different sets of atomic data (AIM, ADAS) a discrepancy shows up. Considering a conservatively estimated error of the AIM data to be a factor 3 and for the ADAS data to be of order 50 % the discrepancy is within the uncertainties of the atomic data. Similar investigations are performed on several high-Z elements (Hf, Ta, Re, Au). The results show the same relation between the 3 introduced evaluation methods. In fig. 3 the cooling factors of tungsten, which have been used for the above analysis of total radiation, are compared. Two ADAS curves are presented; the lower curve corresponds to the calculation in which a limited number of configurations are included, the number constrained by computationl resources. To estimate the 'missing' contribution the data was projected to a 'complete' set by extrapolating the included cross sections to higher transitions with a  $\sigma_{m\to n} \propto 1/n^3$  scaling, where n and m are main quantum numbers. The missing configurations, when included in the population calculation will impact on all excited levels. Therefore the difference between the 'ADAS projected' curve (black ADAS graph in fig. 3) and the

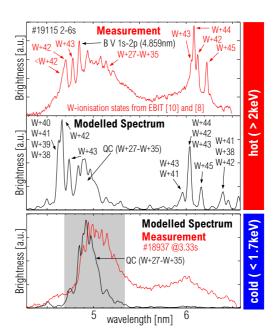
original calculation (red curve) can be used as a good estimate of the error due to using an incomplete set of configurations. The differences between the AIM and ADAS above temperatures of 15 keV are negligible as the amount of continuum radiation becomes comparable to that from line radiation. This vanishing difference means that the maximum tolerable tungsten concentration in a reactor or ITER is not altered by this data revision as only the radiation losses from the hot center of the plasma need to be considered for this. Fig. 4 shows the VUV measured and modelled tungsten emissions around 5 nm at two different background plasma temperatures. As the calibration for these spectra has



**Fig.3:** Cooling factors from [6] and ADAS; ion abundances as guidelines

large uncertainties a detailed comparison of the total emissivities is not shown here. Estimates for the integrated radiated power of the spectra are of the correct order of magnitude.

For the plasma temperatures below 1.7 keV the spectrum is dominated by the quasicontinuum that shows its main feature at  $5.0 \pm 0.3$  nm (gray box). This feature is emitted mainly by ion states between  $W^{+27} \rightarrow W^{+35}$ . The radiating ion states and the wavelengths of their spectral emissions have been documented by high precision EBIT measurements [10]. The wavelength predictions of ADAS for the emissions at the gray box are too low by 0.1 nm-0.2 nm. The ASDEX Upgrade and EBIT measurements show a broader spectral distribution than predicted, because the wavelength spacing in between the emissions of each ion stage is underestimated in the ADAS data. The emissions with wavelengths above 5.4 nm are not understood even when more ion states are included in the modelling. Neither the atomic data nor the EBIT data [10] which considers tungsten ions down to W<sup>+21</sup> can explain the local maximum at 6.0 nm. For a hot background plasma



**Fig.4:** VUV spectra of tungsten for  $T_{e,central} = 1.5 \text{ keV}$  and 3.5 keV

(> 2 keV) spectral lines overlay the quasicontinuum emissions. The relative strengths and wavelengths of these spectral lines agree to a degree that makes an assignment between model and spectrum possible. Although individual lines need to be shifted in wavelength there is a strong correspondance between model and measurement for the envelope features.

#### Conclusion

New ADAS data for high-Z elements was used to model tungsten spectra and was confronted with measurements. The intermediate quality data gave good agreement in the coarse distribution of intensity within each spectrum. The measured total radiated power was predicted correctly while consistency of spectral emissions in comparison to total radiated power was shown for model and measurement. The analysis indicates that the efficiency of tungsten as a radiator has been over-estimated by up to a factor of 3 with the older average ion model data in the 1-10 keV temperature range. Above 15 keV continuum radiation is comparable to line radiation and differences between both data are small.

#### References

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