

M. G. O'Mullane, H. P. Summers, A. D. Whiteford, R. Barnsley,
I. H. Coffey, G. Counsell and S. Loch

Diagnostic Exploitation of Complex Heavy Elements in Tokamak Plasmas

Diagnostic Exploitation of Complex Heavy Elements in Tokamak Plasmas

M. G. O'Mullane¹, H. P. Summers¹, A. D. Whiteford¹, R Barnsley²,
I. H. Coffey², G. Counsell³, S. Loch⁴
and contributors to the EFDA-JET workprogramme*

¹*Dept. of Physics and Applied Physics, University of Strathclyde, Glasgow, UK*

²*Department of Physics, Queen's University Belfast, N. Ireland*

³*Euratom/UKAEA Fusion Association, Culham Science Centre, Abingdon, Oxon. UK*

⁴*Physics Department, Auburn University, Alabama, USA*

* *See annex of J. Pamela et al, "Overview of Recent JET Results and Future Perspectives", Fusion Energy 2000 (Proc. 18th International Conference on Controlled Fusion and Plasma Physics, Sorrento, 2000), IAEA, Vienna (2001)*

“This document is intended for publication in the open literature. It is made available on the understanding that it may not be further circulated and extracts or references may not be published prior to publication of the original when applicable, or without the consent of the Publications Officer, EFDA, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK.”

“Enquiries about Copyright and reproduction should be addressed to the Publications Officer, EFDA, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK.”

ABSTRACT

In future burning plasma experiments, a promising method for the diagnosis of first wall erosion is to detect the onset of emission from nonintrinsic materials embedded in the plasma facing components as they are revealed and enter the confined plasma. Likely high Z species were introduced into JET plasmas by laser ablation. Results from targets of single species (W and Hf) and dual species (W/Hf composite) are presented. The composite target experiment has shown that it is possible to reliably distinguish between emission from near neighbour heavy elements, even with instrument resolutions of $\Delta\lambda/\lambda \sim 0.001$. Forward prediction to power plant conditions necessitates a model of the complex spectra and a system for generating the required atomic data and producing spectral feature emissivity coefficients is described. An important consideration is to enable exploration of different instrumentation so the spectral resolution of the compound features are tuned to the diagnostic capability.

1. INTRODUCTION

There is a re-appraisal of the use of thermally resistant high Z metals as plasma facing components in future burning plasma devices. Heavy species have generally been avoided because of severe radiative power losses in the core plasma and their contribution to the dilution of electrons relative to fuel ions. However recent experience with tungsten ($Z=74$) in Asdex Upgrade[1]. indicates that there is an encouragingly low penetration into the core plasma. Practical power plants are likely to expose both low and high Z species to the plasma. The use of Carbon Fibre Composite (CFC) tiles is at the expense of significant carbon erosion.

As heavy species will not be fully ionised in burning plasmas, they can be embedded into the CFCs and the appearance of their spectroscopic signature used as a diagnostic of the tile's erosion. Rapid identification of these spectra thus has the dual advantages of measuring the carbon erosion rate and of monitoring any tungsten leakage from the divertor into the main chamber.

To exploit these spectra diagnostically requires a different approach than that of interpreting emission from the light ions. The spectra are complex and thus their calculation requires a much larger quantity of atomic data. There are challenges in spectral interpretation, data generation and of data quality. This paper outlines approaches to heavy species spectral analysis and to generating the atomic data and its ultimate condensation to a size for practical diagnostic use. The approach recognizes that theoretical modelling will be necessary to expand the limited experimental spectral data in order to interpret spectra from arbitrary species in varying machine conditions. This implementation is part of the Atomic Data and Analysis Structure (ADAS) project[2]. High Z spectra from Tungsten and Hafnium ablated into JET plasmas are used to test the system.

2. EXPERIMENT

The twin issues of practical spectroscopic detectability and distinguishing between neighbouring elements were addressed in a series of laser ablation experiments in JET. Quiescent L-mode plasmas

were heated with ICRH to give a variety of plasma electron temperatures in the 2 - 8keV range. The JET laser blow-off system delivers a $\sim 8\text{J}$ pulse to the back of a glass target coated with a $5\mu\text{m}$ layer of impurity. The spot size is $\sim 4\text{mm}^2$ and approximately 5% of the 10^{18} ablated particles enter the confined plasma, the rest being lost in the scrape off layer and delivery tube. The rise in radiated power can be substantial, reaching 10MW on occasion, but the plasma and Z_{eff} are not perturbed because, in these plasmas, the injected impurity confinement time is $\sim 250\text{ms}$. Pure hafnium, tungsten, lead and bismuth (Z of 72, 73, 82 and 83) were injected along with composite targets of Hf/W and Pb/Bi. Two types of composite target were tested - a co-deposited alloy and a multilayer built up from $1\mu\text{m}$, layers. The targets were manufactured by Lebow[3].

Figure 1 compares spectral emission in the $40\text{--}70\text{\AA}$ region from W and Hf and composite Hf/W targets. It shows characteristic emission from the $4p^64d^n - 4p^64d^{n-1}4f$, $4p^54d^{n+1}$ ionisation stages[4]. With a grazing incidence (SOXMOS) spectrometer[5]. of wavelength resolution 0.2\AA these near neighbours in the periodic table are distinguishable. Although this instrument is configured in JET with a direct view of the plasma, it is possible to image the plasma via a mirror in a similar fashion to the JET SPRED VUV spectrometer[6]. which would allow its use in an actual power plant.

To discover the proportions of emitting elements from a compound spectra requires a basis set of pure spectra at the same plasma conditions. Figure 1 shows that this is possible in a purely experimental way. A least squares fit of the form

$$\lambda_{\text{comp}} = \lambda_{\text{comp}}^{\text{bg}} + \sum_i p_i \lambda_i^{\text{imp}} \quad (1)$$

where λ_i^{imp} is the experimentally measured spectrum (less any background contribution) of a impurity i , and p_i is the fitted proportion, rapidly converges. Figure 2 shows the sensitivity of the problem where the same spectral range of tungsten at different temperatures shows significantly different behaviour.

Therefore there are major drawbacks to relying on a purely empirical scheme: the pure spectra basis functions must be taken in the same conditions and hence forward predictions to burning plasma conditions are not possible.

The fit of the pure materials spectra to that of the composite target highlights a difference in the target properties with the multilayer demonstrating a more tungsten-like character than the alloy. In fact target differences are a general problem in ablation studies with, eg., lead giving cleaner spectra than bismuth. Such variation in impurity delivery and the short confinement time means that ablation studies are only a part of assessing the suitability of using high Z materials embedded in PFC tiles as an erosion monitor. However the small quantities introduced were easily detectable with XUV and VUV instrumentation and the crystal survey instrument was particularly sensitive ($2\text{--}7$ and $10\text{--}35\text{\AA}$) and frequently saturated.

3. COMPLEX ATOM MODELLING

For fusion spectroscopic diagnostics the focus of fundamental cross section calculation and of population modelling has been on the light ions up to neon. For these ions a comprehensive generalised collisional-radiative model considering all low lying states is feasible. The population of an excited level in an ion, N_j , is driven by excitation from the dominant metastable states (which include the ground state) and by recombination from the metastables of the adjacent ion.

Collisional and radiative processes between all excited levels redistribute the populations. The excited levels are in quasi-static equilibrium with the metastables,

$$N_j \equiv \sum_{\sigma=1}^{M_z} F_{j\sigma}^{\text{exe}} N_e N_{\sigma} + \sum_{v=1}^{M_{z+1}} F_{jv}^{\text{rec}} N_e N_v^+ \quad (2)$$

where metastables are denoted by Greek indices. The $F_{j\sigma}(T_e, n_e)$ are the effective contributions to the excited populations. The dominant metastable ion densities, N_p , come from a dynamic ionisation balance calculation (the collisional-radiative model also delivers these source coefficients). The emissivity in a spectral line is then,

$$\epsilon_{j \rightarrow k} = A_{j \rightarrow k} N_j \quad (3)$$

with the associated excitation photon emissivity coefficient

$$\text{PEC}_{\sigma, j \rightarrow k}^{\text{exe}} = A_{j \rightarrow k} F_{j\sigma}^{\text{exe}} \quad (4)$$

Methods for generating photon emissivity coefficients are well established using mature codes, such as those in ADAS. They are used as part of the routine analysis of spectra at JET.

High Z ions, such as molybdenum and tungsten, will not be fully ionised even in future burning plasmas and have many more levels than the simpler systems due to partially filled inner shells. Relativistic effects ensure that the atomic structure is in intermediate coupling which also increases the quantity of data over LS coupled systems. Their spectral lines will be dispersed over transition arrays and will appear grass-like or as a quasi-continuum.

An issue is to enable exploitation of complex spectra for diagnostic purposes; that is to be able to manipulate the atomic data in a simple way without losing any of the sophistication of the modelling. Therefore the theoretical emission data must be associated with the diagnostics available; in practice it must be keyed to the wavelength range and resolution of a particular instrument.

For each ion introduce a new coefficient, the envelope feature photon emissivity, which is analogous to the photon emissivity of an individual line but is a composite feature arising from many individual lines. It is function of a digitised wavelength interval as well as temperature and density. For a wavelength interval, $[\lambda_0, \lambda_1]$ divided into N pixels, and assuming that each line has a normalised emission profile, $\phi_{j \rightarrow k}(\lambda)$, define

$$\text{FPEC}_{\sigma, i}^{\text{exe}[0,1]} = \sum_{j,k; \lambda_{j \rightarrow k} \in [0, 1]} \text{PEC}_{\sigma, j \rightarrow k}(T_e, N_e) \int_{\lambda_{j \rightarrow k}}^{\lambda_{j \rightarrow k}'} \varphi_{j \rightarrow k}(\lambda) d\lambda \quad (5)$$

By adopting a minimal broadening (Doppler with an ion temperature equal to the electron temperature used to calculate the PECs) this feature coefficient can be easily convolved with instrument functions or power filters.

The ionisation balance between adjacent stages, particularly as a shell such as $4d^n$ ionises, is weakly dependant on temperature because of the very similar ionisation potentials. This effect offers a further economy in the number of derived coefficients required. A set of FPECs bundled over groups of ionisation stages, along with a concomitant bundling of ionisation and recombination rates, permits transport modelling analysis of such spectra.

The calculation of the FPECs and other data requires very substantial computer power and time but diagnostic use of the final derived feature coefficients requires only a simple extension of existing interpretation techniques. The analysis technique of fitting measured spectra to a model which distinguishes between a calculated feature and ‘ordinary’ emission lines, which may by chance lie in the observed region, is well established.

4. COMPUTATIONAL IMPLEMENTATION

The computational needs for exploiting these complex spectra as a plasma diagnostic fall into two areas viz. generating the atomic data and condensing it in a fashion suitable for routine use. A guiding principle is to maintain a strong link with a given instrument. The framework is implemented in three ADAS codes.

An interactive code sets up the drivers for the datasets for the large fundamental cross-section calculations. Electron promotion rules from the ground stage of each ion are setup by choosing different valence shells, Δn rules, restrictions on the configuration complex and whether inner shell promotions are permitted. Configuration average energies are calculated to determine and display the mean wavelengths of the transitions as a guide. At this stage the wavelength of the spectrometer is used in order to determine which configurations need to be treated in a resolved intermediate coupling picture and which to treat as configuration average for the population calculation.

Even with this reduction, a large number of levels within an ionisation stage is likely. Also there will generally be many ionisation stages as the isonuclear mean wavelength of the transition arrays changes slowly. For baseline data generation, Cowan’s structure code[7]. is employed on a parallel machine. This gives intermediate coupling Born effective collision strengths which are then assembled in specific ion files (ADAS format : adf04) consisting of resolved levels which give rise to emission within the spectrometer’s range and configuration average values for the rest. It must be noted that this is the first level of layered calculations for complex species. It allows for the inclusion of more sophisticated methods, such as distorted wave or even R-matrix, to target individual ionisation stages of interest.

The final stage is the generation of the envelope feature photon emissivities ($FPEC(T_e, n_e, \lambda)$) using a modified version of the collisional-radiative code in ADAS. Hence the vast amount of atomic data is condensed to a usable set of coefficients, an example of which is shown in Fig.3.

5. CONCLUSION

This paper has shown how heavy species impurities can be detected and distinguished using standard spectrometers in current machines. The composite spectrum of more more than one heavy species can be constructed from a set of single species basis spectra. A theoretical framework has been described to expand the experimental work to all future machines and species. Baseline data production is underway.

ACKNOWLEDGEMENTS

This work has been conducted under the European Fusion Development Agreement and is partly funded by Euratom and the UK Department of Trade and Industry.

REFERENCES

- [1]. R. Neu et al., Plasma Phys. Control. Fusion 44, 811, (2002)
- [2]. H. P. Summers, The ADAS User Manual - version 2.4 (2001), <http://adas.phys.strath.ac.uk>
- [3]. Lebow Company, 5960 Mandarin Ave., Goleta, CA 93117, USA.
- [4]. R. Radtke et al., Phys. Rev. A, 64 012720, (2001)
- [5]. J. L. Schwob et al., Rev. Sci. Instrum. 58, 1601, (1987)
- [6]. R. Barnsley et al., These Proceedings.
- [7]. R. D. Cowan, Theory of Atomic Structure and Spectra, University of California Press, (1981).

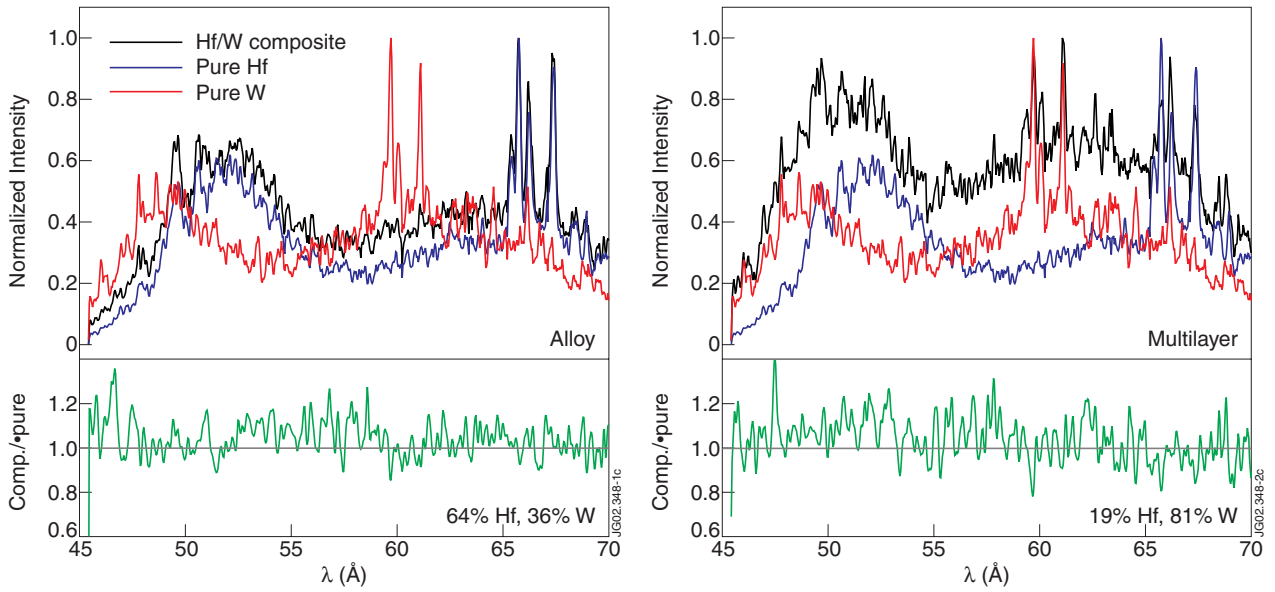


Figure 1: Overlay of spectra from composite target and the pure spectra into identical plasmas; Alloy target (top) and multilayer target (bottom). The second pane in each figure is the ratio of compound to pure components from a simple fit.

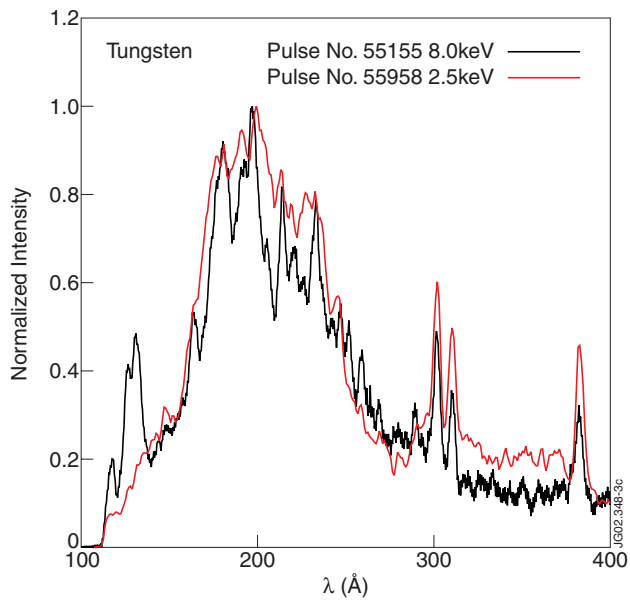


Figure 2: Overlay of normalised spectra (including sensitivity adjustment) from tungsten ablated into different temperature plasmas.

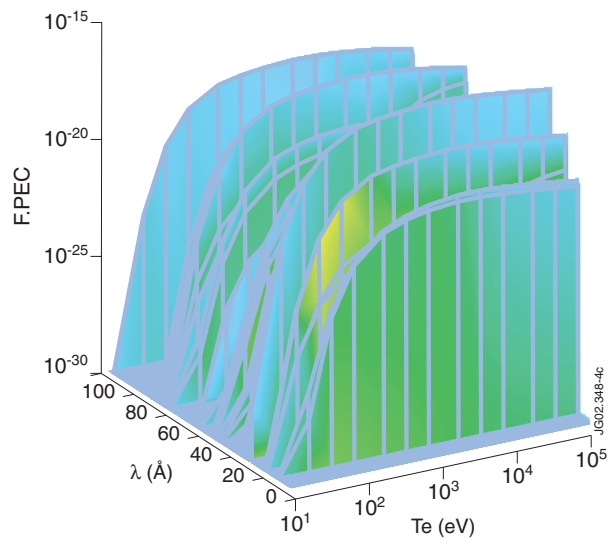


Figure 3: Emission from Hf^{28+} (Ru-like - $3d^{10}4s^24p^64d^8$) in the 10–120Å region assuming a 1Å resolution. Note the strong temperature variation over a range likely in a tokamak burning plasma.