International Atomic Energy Agency

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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Second Technical Committee Meeting on Atomic and Molecular Data for Fusion

Fontenay aux Roses, 19-22 May 1980

REPORTS OF THE WORKING GROUPS

Prepared by
K. Katsonis
Atomic and Molecular Data Unit
Nuclear Data Section

October 1980

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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REPORT OF THE WORKING GROUP ON INTERNATIONAL COOPERATION

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Introduction

Since the Culham meeting in 1976*, the awareness of atomic physics research needs for fusion applications and the volume of data produced for such applications has significantly increased. The present meeting fulfilled a useful function in summarizing the current fusion requirements and the status of the A + M data research work that has been performed since the Culham meeting.

A. Assessment of data requirements and Status

In order to keep pace with the fast moving data requirements for fusion, and the progress in A + M data research for fusion, it is recommended that the Agency continue to review the A + M data requirements for fusion, as well as the status and availability of the required data through specialists meetings. In particular, it is proposed that the IAEA:

(i) continue convening international meetings on A+M data for fusion of the Culham or Fontenay-aux-Roses type every three years;

(ii) consider holding smaller international specialist meetings on specific aspects of A + M data for fusion of current interest (such as data for plasma modelling codes, surface interaction data, charge exchange, etc. ..) whenever necessary.

(iii) publicize the results of these meetings in the form of concise reports to the A + M physics and fusion communities.

*) IAEA Advisory Group Meeting on Atomic and Molecular (A+M) Data for Fusion, held at the UKAEA Culham Laboratory, Abingdon, UK, 1-5 November 1976; Proceedings issued as Technical Document IAEA-199, 1977.

It was recommended that the coverage of fusion technology by the IAEA A + M data programme be broadened to cover those aspects related to A + M physics of current interest in magnetic and inertial confinement devices.

B. Bibliographic Data

B.1 International Bulletin on Atomic and Molecular Data for Fusion

The meeting acknowledged the IAEA Bulletin and recommended that it be continued to be published on a quarterly basis. Production of the Bulletin requires a broad range of technical expertise and excellent specialized library facilities. It will be difficult for the IAEA to maintain on its staff the necessary range of expertise. It is therefore recommended that the Agency adopt a general policy to delegate portions of the Bulletin to other institutions. Where possible, the associated institutions should do the necessary searching of the literature and also make the judgements concerning fusion relevance. Particular fields where this delegation is possible and desirable are (a) surface data, (b) spectroscopic data, and (c) plasma diagnostic data. The Agency should insure that the uniform character of the Bulletin be maintained.

B.2 CIAMDA - Bibliographic Index to A+M collision data

The meeting acknowledged the announced publication of the first edition of CIAMDA, and recommended that updates of this bibliographic data base be published every two years.

In addition it was suggested that the CIAMDA data base be accessible by users for selective retrievals between publications.

B.3 Other data indices

The meeting noted that CIAMDA does not contain fusion-oriented atomic structure and surface data references, and recommended that IAEA investigate the possibility to have such indices produced with a specific information cut-off reflecting fusion needs.

C. Numerical A+M data

C.1 IAEA Activities

The meeting recognized that the principal objective of the IAEA A+M data programme is the establishment of an international data centre service to provide evaluated A+M data to the fusion research community. It was therefore recommended that the coordination of the production and dissemination of A+M data should be the area to receive the greatest emphasis. Evaluated data produced by specialists in the field should be reviewed by a small group of experts for acceptance into the IAEA data file.

The meeting specifically recommended that the IAEA A+M Data Unit should not collect and disseminate unevaluated data. In order to facilitate the collection and inter-centre exchange of evaluated data, it is recommended that common computer formats for the exchange of evaluated A+M data between the A+M data centres be defined.

C.2 Production of A+M data for fusion

In view of the large need for new and improved A+M data for fusion, the IAEA is asked to use the means and the procedure at its disposal to support the production of the required A+M data.

In this context it is recommended that the IAEA initiate some cooperative research programmes concerned with the measurement, calculation and evaluation of A+M data, whereby emphasis should be given to data most urgently needed, as identified by this meeting. Such programmes would generally associate on a voluntary basis several laboratories from a broad spectrum of countries. Within these programmes the Agency should support research in countries without extensive fusion programmes.

It was also noted that research groups from developing countries could make valuable contributions to these efforts. It is therefore recommended that the IAEA support fellowships for scientists from such groups to participate in the work of well-established research groups and data centres.

As the above-suggested contribution by the IAEA can only be minimal, in view of the large effort required, the meeting felt that a much larger support of fusion-oriented A+M physics research would be necessary, particularly in those Member States and Organizations which have on-going fusion programmes.

In order to assist Member States and Organizations to focus their A+M physics research toward the requirements of the fusion community, it is recommended that the IAEA try to provide a summary of the most urgent A+M data requirements for fusion as outlined in section "A" of this report, at regular intervals. This information would be circulated to the A+M physics and fusion research communities. Specific data requirements (e.g., atomic or molecular species, data type, energy range, accuracy, specific purpose) would be indicated. An overview of such data requirements is incorporated in the other working group reports from this meeting.

REPORT OF THE WORKING GROUP ON ATOMIC AND MOLECULAR DATA FOR PLASMA MODELLING AND DIAGNOSTICS

Working Group Members

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Raimbault, Dr. P.
Salzborn, Prof. E.
Suckewer, Dr. S. (Chairman)
Van Regemorter, Dr. A.
Volonte, Dr. S.
*Wiese, Dr. W.L.
Winter, Dr. H.

The group worked in two sections devoted to atomic collision data and to atomic structure and wavelengths data. The second section was chaired by Dr. W. L. Wiese; the names of the members of the group working in Section II are marked by asterisks (Dr. N.J. Peacock participated in both sections). Consequently this report is separated into two parts.

In Part I. after a short introduction (I.A.) a list of the collision data requirements is given (I.B.) including the necessary justification. An additional list of specific reactions related to neutral beam heating and alpha particle diagnostics is given under I.C.

Part II. comprises an introduction (II.A) and a list of the structure and wavelength data requirements (II.B.). The assessment of data compilations as compared to the requirements and recommendations to IAEA are given in II.C., II.D. correspondingly.

I. ATOMIC COLLISION DATA

I.A. Introduction

a) Progress since 1976

There has been considerable progress in collision data relevant to fusion since the 1976 meeting in Culham.

The first item is that the issue of beam trapping by impurities has been resolved. The relevant cross sections have been measured and calculated, and general scaling formulas and data are available. The results for 60 keV/a.m.u. hydrogen atoms are that charge exchange ($H^o + A^{q+} \rightarrow H^+ + A^{(q-1)+}$) is the dominant process, and neutral beams can penetrate JET or TFTR sized plasmas even if impurities are present in the experiment.

The second development has been that radiation losses and spectra from medium (Fe) and heavy (Mo, W) metals have been calculated and heavy metal radiation has been identified as one of the major energy loss mechanisms on a large number of fusion experiments (ORMAK, PLT, DITE, T-10, DIVA, JFT-2 etc.). Several methods were applied to decrease the plasma edge temperature, and in this way strongly decrease influx and concentration of metals from limiter and wall. Further decreasing the radiation from the plasma core by using a carbon limiter made it possible to obtain the encouraging high temperature results on PLT with neutral beam heating.

A third development is a general improvement in electron collision data followed by new and improved plasma diagnostics. The application of less approximate excitation rates has increased the accuracy of the measurement of the radial density profiles for various charge states. Improved ionization and recombination rates have led to a more reliable interpretation of these impurity density profiles. The identification of forbidden lines for highly ionized iron and titanium has allowed the measurement of the ion temperature profile by Doppler broadening in the central region of high temperature ($T_e \gtrsim 2$ keV) plasmas as well as toroidal plasma rotation and high - z impurity concentrations. The ratio of the intensities of dielectronic satellite lines to resonance lines for iron have been used to measure electron temperatures in hot ($T_e \gtrsim 2$ keV) plasmas. Inner shell excitation satellite lines have also been used to measure relative impurity charge state radial profiles. Charge exchange of oxygen and carbon by introducing a neutral hydrogen beam has allowed the measurement of the central density of a fully stripped impurity. Charge exchange also has been recognized as a mechanism of changing the ionization equilibrium of the impurity ions during neutral beam injection and in this way increasing plasma radiation losses.

There was also recognition of the importance of the plasma modelling for a better understanding of the radial distribution of impurity stages of ionizations. It was found that the deviation from the corona equilibrium model can be significant, especially during neutral beam injection.

There has been significant progress since the last meeting in the development of powerful neutral beam injection systems, including the reduction of undesired molecular ions produced by the ion source. Some progress has been made in modelling these sources.

Another new development has been the measurement of electron impact ionization cross sections for a number of partially stripped ions and the identification of the importance of the excitation-autoionization mechanism as a contributor to the total ionization cross section (especially for higher ionization stages).

b) New needs

In the light of progress since the 1976 Culham meeting the atomic and molecular collision data needed for fusion research have been slightly changed. Partially as a result of the beam trapping work, calculations and measurements have been performed on the ionization balance of impurities due to charge transfer between multi-charged impurity ions and neutral hydrogen (primarily from neutral beams).

This has led to interest in low velocity cross sections between neutral hydrogen and partially ionized ions, a process important at the edge and in divertors. Data about the specific excited states (n,ℓ) resulting from charge exchange collisions ($H^0 + A^{q+} \rightarrow H^+ + A^{(q-1)+}(n,\ell)$) are important for using the charge transfer to measure the density of A^{q+}.

There is a continued interest in improvements in the electron collisional recombination, ionization, and excitation cross sections of partially ionized impurities. Accurate rates should also be made available to be able to improve the calculations of power loss rates due to impurities. It has to be pointed out that atomic physics investigators should bear in mind that atomic collisions in tokamaks occur in magnetic fields of 1 to 10 T so that there is the possibility of subsequent field ionization by Lorentz forces and in addition there may be fluctuating electric fields up to 1000 V/cm.

A development which grew out of the INTOR study has been the recognition of the importance of electronic and atomic processes at the plasma edge and in divertors. A quantitative understanding of atomic and molecular hydrogen, helium, and impurity atomic processes at low temperatures will be essential to the design of a reactor-like experiment.

The optimum design of neutral beam systems will require accurate knowledge of a wide variety of collision data for primarily low energy atomic hydrogen, molecular hydrogen and impurity. Hydrogen always stands also for its isotopes.

The development of negative hydrogen ion sources is an important effort with significant atomic physics needs.

The measurement of the confinement of fusion produced alpha particles will be important for any fusion experiment. The development of such a diagnostic requires the measurement and calculation of several cross sections now not known, such as for Li^0 colliding with He^{++}, and the construction of devices yielding high currents of He^- and Li^-.

The committee did not have the relevant expertise to make specific recommendations on the atomic data required for inertial confinement fusion. However, it recognises that this approach to Controlled Thermonuclear Fusion Research requires a quite different set of priorities for basic data. Radiation transport, plasma degeneracy and polarisation, collective processes, and slowing down of thermonuclear reaction products are some of the topics which suggest themselves for study.

I.B. Data requirements and justification for atomic and molecular collision data

(REQUIREMENTS)	(JUSTIFICATION)
1. Species	
Hydrogen, H, including isotopes D, T.	Basic plasma constituents.
Carbon C, Oxygen O, Fluorine F, Boron B, Silicon Si, Chlorine Cl, Aluminum Al, Titanium Ti, Iron Fe, Nickel Ni, Chromium Cr, Nitrogen N.	Used as or contained in materials for first wall.
Molybdenum Mo, Tungsten W, Copper Cu, Zirconium Zr.	Used in limiters, ion sources and other external devices, but less likely to be found in the plasma in advanced designs.
Helium He.	Ash, α-particle diagnostics.
Neon Ne, Argon Ar, Krypton Kr, Xenon Xe.	Impurity diagnostics and possibly for burn temperature control.
Lithium Li and Caesium Cs (and other alkali metals).	Active beam diagnostics (includes Li ion or neutral beam) and H^- beam formation, divertor materials.
Molecular hydrogen isotopes and low hydrocarbons and hydroxyls.	Boundary plasma, start-up, neutral beam injection, wall chemistry.

(REQUIREMENTS)	(JUSTIFICATION)
2. Electron excitation	
Transitions mainly from ground states, also metastable states and some lower excited states; inner-shell and double excitation for all ionization stages of interest up to an ionization potential of approximately 50 keV. Energy range: from threshold to at least 10 times threshold. Accuracy: $\pm$ 20 % High priority.	Plasma modelling (power loss, particle transport, particle concentration). Diagnostics (including inner-shell satellite lines for ion abundance ratios).
3. Electron ionization	
Same species and energy range as for 2.	Same reasons as for 2.
4. Excitation of impurity ions by H^+, D^+, T^+ and He^{++}	
Energy range: hydrogen isotopes up to 200 keV/a.m.u. He^{++} up to 3.5 MeV. Accuracy: factor 2 Low priority.	Augments total excitation rate for $\Delta n = 0$ transitions, especially those within the ground configuration.

(REQUIREMENTS)	(JUSTIFICATION)
5. Ionization of H^o and D^o by H^+, D^+ and T^+	
Energy range: up to 200 keV/a.m.u.	Beam penetration.
Accuracy: $\pm$ 20%	
High priority.	
6. Electron capture	
(a) $A^{q+} + H^o \rightarrow A^{(q-1)+} + H^+$	Modifies recycling, ionization balance and power loss.
(H stands for all hydrogen isotopes; A^{q+} is the impinging ion)	Diagnostics; in this case the quantum numbers (n, ℓ) of the final impurity ion state are important.
Energy range: 1 eV to 200 keV/a.m.u.	Beam penetration
Accuracy: $\pm$ 20%	
High priority, in particular for low energies.	
(b) $H^+ + A^{q+} \rightarrow H^o + A^{(q+1)+}$	Sources of hydrogen within the plasma.
(H stands for all hydrogen isotopes; A^{q+} is the impurity ion)	
Energy range: 1 to 20 keV.	

(REQUIREMENTS) (JUSTIFICATION)

Accuracy: factor 2

Low priority.

(c)

$$He^{2+} + X^{q+} \rightarrow He^{+} + X^{(q+1)+}$$

$$He^{2+} + X^{q+} \rightarrow He^{o} + X^{(q+2)+}$$

α-particle energy transfer and helium recycling. Helium diagnostics (including active beam).

(X stands for hydrogen, helium and impurity atoms)
Excited states of hydrogen up to n = 10 and metastable helium should be included.

Energy range: 1 eV to 1 keV and 0.5 to 3.5 MeV.

Accuracy: $\pm$ 20%

High priority.

7. Electron - ion recombination

(a) Radiative

Same reasons as for 2.

For all plasma ions, with (n,ℓ) distribution

Energy range: 0.1 to 5 times the ionization potential of the ion.

(REQUIREMENTS) (JUSTIFICATION)

Accuracy: ± 20%

High priority.

(b) Dielectronic

All relevant impurity ions, with (n,ℓ) distribution, in plasmas with $n_e \simeq 10^{12}$ to 10^{15} cm^{-3} (magnetic field strength ≃1 to 10 T).

Energy range: as for 7.(a).

Accuracy: ± 20%

High priority.

Same reasons as for 2; also measurement of electron temperature using dielectronic satellite lines.

8. Electron - molecule collisions

(a) Dissociation (cross section and product description)

Neutral and ionized molecules listed in 1., including effects of vibrational excitation.

Energy range: 0.1 to 150 eV.

Accuracy: ± 20%

High priority for hydrogen isotopes.

Ion source and beam lines, recycling, divertors.

(REQUIREMENTS)	(JUSTIFICATION)
(b) Excitation and ionization	Ion source and beam lines, edge cooling, divertors.
Same requirements as for 8.(a).	
Energy range: 1 to 150 eV.	
Accuracy: factor of two	
Low priority.	
(c) Dissociative attachment	Ion source (and beam lines).
$e^- + H_2^+ \rightarrow H^- + H^+$	
$e^- + H_3^+ \rightarrow H^- + H_2^+$	
Same requirements as for 8.(a).	
Energy range: 1 to 150 eV.	
Accurancy: factor of two	
High priority.	
(d) Collisional electron detachment	Ion source (and beam lines).
$e^- + H_2^- \rightarrow e^- + H_2^o + e^-$	
Requirements and energy range as for 8.(c).	

(REQUIREMENTS)	(JUSTIFICATION)
(e) Dissociative electron attachment for electronic ground and excited states $e^- + H_2 \rightarrow [H_2^-] \rightarrow H(n,\ell) + H^-$ Also the dependence of the cross sections on the vibrational quantum number υ may be important.	Ion source (and beam lines).
(f) Polar dissociation $e^- + H_2 \rightarrow H^+ + H^- + e^-$	Ion source (and beam lines).

9. Ion - molecule collisions

(a) High energy (10 to 200 keV/a.m.u.) H^+, H_2^+, H_3^+ with H_2 or other neutralizer gas (H stands for all hydrogen isotopes).	(Related to neutral beam injection)
(i) leading to fast H atoms	Beam neutralization
(ii) leading to fast excited atoms	H_α and H_β (Doppler shifted diagnostics).
(iii) leading to slow recoil atoms	As for (ii) but not Doppler shifted.

(REQUIREMENTS)	(JUSTIFICATION)
(b) Low energy (1 to 100 eV)	
(i) H^+, H_2^+, H_3^+ with H_2, H^- leading to H_3^+ formation and destruction and mutual neutralization.	Ion source modelling, recycling, divertors.
(ii) Formation and destruction of hydrocarbons and hydroxyls.	Recycling; wall chemistry.

<u>I.C. Specific reactions related to neutral beam heating and alpha particle diagnostics.</u> (H stands also for D)

(REACTION)	(REQUESTED QUANTITY)	(ENERGY)
Fast impurities (Cu, Mo, W,..) on noble gases producing x-rays	L (M where possible) x-ray cross sections from projectiles	20-200 keV
H^+ on noble gases producing x-rays	L x-ray cross sections from target gas	20-200 keV
$H^o + H_2 \rightarrow H^*$	H_α, H_β, production	10-200 keV
$H_3^+ + e^- \rightarrow H_2^+ + H + e^-$	cross sections for H_2^+ production	0.1-5 eV
$H_2^+ + H_2 \rightarrow H_3^+ + H$	Dependence on vibrational states of H_2^+, H_2	0.1-5 eV
$H^- + H_3^+ \rightarrow H + \ldots$	Destruction of H^-	0.1-5 eV
Fast impurities (C, O, Cu, Mo, W, ...) in H_2	Electron capture loss, equilibrium fraction of fast impurities	10-200 keV
$He^* + p \rightarrow He^+, He^{++} \ldots$	σ_{0*1}, σ_{0*2}	0.5-3 MeV
$He^- + A^o \rightarrow He^o$ or $He^* + \ldots$	Ground state and metastable yield	0.5-3 MeV
$He^* + He^{++} \rightarrow He^o$ or $He^* + \ldots$	σ_{20}, σ_{20*}	0.01-5 MeV
$Li^o + He^{++} \rightarrow He^o + \ldots$	σ_{20}, σ_{20*}	0.01-5 MeV
$Li^- + A^o \rightarrow Li^o + \ldots$	Neutral yield $\sigma_{\bar{1}0}$	1-6 MeV
$Li^+ + A^o \rightarrow Li^- + \ldots$	Li^- yield	1-20 keV
$HeH^+ + A^o \rightarrow He^o + \ldots$	He^o yield	0.5-4 MeV

II. ATOMIC STRUCTURE AND WAVELENGTHS DATA

II.A. Introduction

The working group has examined the status of spectral atomic data with respect to the needs of thermonuclear fusion programmes, and feels that the earlier 1976 consultants report to the IAEA*by a similar working group is in many respects still applicable. The format of that report was found to be very useful and therefore has been largely maintained. However, as shall be seen below, many significant changes in the data needs and shifts in the priorities of the data have occurred. There are still major gaps in the data and needs are immediate as well as long term. Currently of main importance are (a) spectral radiation data for temperature and density diagnostics; (b) data for heavy ion impurities in high-temperature plasmas, since these lead to major radiative energy losses; and (c) spectral data for studies of the plasma edge region, for example, by fluorescence spectroscopy. The Committee has not given proper attention to the data needs for inertial fusion approaches because of lack of relevant expertise in this field. For the same reason, molecular structure data were excluded, although the Committee recognizes that they are important. For requirements on molecular spectra the list appearing in issue no. 5 (1978) of the IAEA A+M Data for Fusion Bulletin should be consulted.

The report has been subdivided into three topics, namely

Data requirements and justifications.
Status of the major existing data compilations.
Recommendations to IAEA.

For each of these topics the data areas of wavelengths and energy levels, atomic transition probabilities and line shapes were addressed in detail.

II.B. Data requirements and justification

1. Wavelength data and energy levels

	(REQUIREMENTS)	(JUSTIFICATION)
1.1.	Identification of the spectra of moderately and highly ionized impurity elements in spectral	Important for diagnostic purposes, for example via measurement of

*) See report IAEA-199

	(REQUIREMENTS)	(JUSTIFICATION)
	regions conveniently accessible to experiment. Currently of major interest are C, N, O, F, Al, Si, Cl, Ar, Ti, Cr, Fe, Ni, Cu, Zr, Kr, Mo, Xe, W. This specifically includes data for forbidden lines in ground state configurations; ions with $2p^n$ ($1 \leq n \leq 5$) configurations are especially important.	Doppler widths of lines in the visible, normal incidence ultraviolet, or x-ray region.
1.2.	Identification of the most intense lines in the spectra of selected elements heavier than nickel (especially Kr, Mo, Zr, Xe) in all stages of ionization, for all elements used as wall and limiter materials in fusion devices.	Wavelengths of these lines, mostly not yet available, are needed for basic identification of the presence and ionization stages of impurities.
1.3.	Detailed identification of spectra arising from transitions involving the most important configurations for all the above listed impurity elements encountered in fusion research, as well as for neighbouring ions to carry out isoelectronic sequence studies. These analyses should specifically include metastable levels.	Detailed knowledge provides valuable general consistency checks, e.g., by regularities along isoelectric sequences, and support for other atomic data.

1.4 Attention should also be paid to the following, more specific points:

i)	Wavelengths of K and L x-ray transitions of highly ionized impurity elements as a function of ion charge state.	Needed for independent determination of stage of ionization of impurities.
ii)	Wavelengths of dielectronic recombination "satellite" lines.	Needed especially for diagnostics with x-ray spectroscopy for very high temperature (several keV) plasmas.
iii)	Energies for autoionizing states.	

	(REQUIREMENTS)	(JUSTIFICATION)
iv)	Ionization energies.	
v)	Fine structure in impurity ion spectra.	Important for identification of forbidden transitions.

2. Atomic transition probabilities

	(REQUIREMENTS)	(JUSTIFICATION)
2.1.	Determination of the atomic transition probabilities of the above listed impurity elements for both low (neutrals to fifth stage of ionization) and highly stripped ions.	Required for estimation of excitation rates used in plasma modelling; for selecting the most suitable lines for impurity diagnostics, including spatial and temporal distribution of species in a plasma; for applying the branching ratio calibration technique.
2.2.	Autoionization probabilities.	Knowledge is required for calculation of dielectronic recombination coefficients, ionization balance, radiation energy losses, and plasma modelling.
2.3.	Atomic transition probabilities for forbidden lines of highly ionized species as specified under 1.1, with relatively long as well as short wavelengths.	Needed for selecting suitable lines for Doppler ion temperature diagnostics; also required for plasma modelling (e.g., for calculating the population densities of excited levels of ions having metastable levels and hence predicting their spectra, for power loss, etc.).

(REQUIREMENTS)	(JUSTIFICATION)
3. Line shapes	
3.1. Line profiles, especially Stark broadening parameters, in which such effects as ion dynamics, plasma polarization, etc., are considered.	Plasma diagnostics; solution of radiative transfer problems especially for high density plasmas; plasma modelling. Note that also collective plasma effects may influence the line profiles.
3.2 Influence of strong magnetic and electric fields on line profiles, emission spectra, and dielectronic recombination.	Plasma diagnostics, solution of radiative transfer problems especially for high density plasmas; plasma modelling.

II.C. Assessment of data compilations as compared to requirements

In the field of wavelengths and atomic energy data compilations, the following principal tabulations are available:

- Atomic Energy Levels, Vols. 1, 2, 3, 4, published by the NBS Washington, 1949, 1952, 1959, 1978, and supplements on C I - C VI, N I - N VII, O I, H I, D I, T I, Si I - Si IV. Also, a new series of NBS compilations appearing in J. Phys. Chem. Ref. Data: Na I - XI, Mg I - XII, Al I - XIII, K I - XIX, Ca I - XX, Sc I - XXI, Ti I - XXII, V I - XXIII, Cr I - XXIV, Mn I - XXV, Fe I - XXVI.

- Revised Multiplet Tables, published by the NBS, Washington, 1945.

- Nat. Stand. Ref. Data Ser. 68 (1980), NBS (spectral line tables for 45000 lines).

- Atomic and ionic emission lines below 2000 Å, H through Kr, R.L. Kelly and L.J. Palumbo, Naval Research Laboratory, Washington, 1973.

- Atomic emission lines in the near ultraviolet; Hydrogen through Krypton, by R.L. Kelly, NASA Techn. Memorandum 80268 (1979).

- Wavelengths and Classifications of Emission Lines, Z$<$28, by B.C. Fawcett, Atomic Data and Nuclear Data Tables, 16, 135-164 (1975).

Other useful publications are:

- Bibliographies on atomic energy levels and spectra, through June 1979, NBS, Washington.

- Critical bibliography by Prof. Edlen, Lund University, published in the book "Beam-Foil Spectroscopy", I.A. Sellin and D.J. Pegg Eds., Plenum Press, 1976.

- 'Atomic Energy Levels and Grotrian Diagrams', Vol. I, H through P XV; addenda; Vol. II, S through Ti XXII, by S. Bashkin and J.O. Stoner, Jr., North-Holland, Amsterdam, 1975; 1978; 1978.

- 'Grotrian Diagrams for highly ionized iron, Fe VIII to Fe XXVI', by K. Mori, M. Otsuka, and T. Kato, Atomic Data and Nuclear Data Tables, 23, 195 (1979).

In the field of atomic transition probabilities the following principal tabulations are available:

- 'Atomic Transition Probabilities', Vol. I (H through Ne), Vol. II (Na through Ca) published by NBS, Washington (1966 and 1969); Sc, Ti (1975); V, Cr, Mn (1978); Fe, Co, Ni (1980) (Sc through Ni published in J. Phys. Chem. Ref. Data).

These tabulations are being complemented by the NBS bibliographies on Atomic Transition Probabilities, NBS Spec. Publ. 505, and Supplement I (1980). In the field of line shape data the following principal tabulation exists: 'Spectra Line Broadening by Plasmas'; by H.R. Griem, Academic Press, 1974. This book is complemented by the NBS - bibliography on Atomic Line Shapes and Shifts, NBS-Spec. Publ. 366 and Suppl. I, II and III (1972, 1974, 1975, 1978).

It is the opinion of the members of the working group that with respect to the requirements for Fusion Research the aforementioned compilations contain the following serious shortcomings:

- The four major atomic energy data compilations are rather incomplete with respect to the highly ionized heavy atoms. Furthermore, the book of Bashkin and Stoner only deals with the light elements up to titanium (Vol. I and II), and the work of Kelly and Palumbo goes up to krypton and deals only with wavelengths in the vacuum or near ultraviolet region.

Furthermore, these latter compilations rely to a large part on the earlier mentioned atomic energy level compilations.

- Similarly, in the field of atomic transition probabilities the two major NBS compilations of 1966 and 1969 are seriously deficient on highly ionized species. Most of the data on such ions have been obtained since then.

- On the subject of line shapes, the book of Griem only contains data for neutral and singly ionized species.

II.D. Recommendations to IAEA

1. Wavelength Work and Compilations

Much further line identification work as well as compilations for highly ionized species are needed. The description of atomic energy levels in terms of their composition as adopted by the National Bureau of Standards should become standard for the sake of easy comparison of data from different sources.

2. Determination of atomic transition probabilities

In this area the most promising approaches for determining data - theoretical calculations, emission, absorption and hook methods, and beam foil spectroscopy - should be vigorously applied. For low stages of ionization of heavy elements which are important for plasma edge studies, experiments should be the main data producer while advanced calculational methods should provide the bulk of the data for the high ions, with experimental work providing mainly key check points. Since experiments are now approaching the area of very highly ionized species of primary interest for fusion plasma diagnostics, special efforts should be made to proceed in this direction. Also, full use should be made of systematic trends and regularities in atomic oscillator strengths. It is very desirable that the data have high accuracy, approaching the $\pm$ 10% level.

3. Compilation of atomic transition probabilities

The compilations need to be updated and extended to include all ionic species of interest to the fusion research programme. Especially important is an update of the tabulations of the principal light element impurities, C, N, O, Al and Si, which are now ten and more years old.

4. Line shapes

Theoretical and experimental work should be concentrated on two specific subjects:

- Determination of Stark broadening parameters for highly ionized species, which are especially needed for high-density plasma generated by lasers.

- Influence of strong magnetic and turbulent electric fields on the profiles of Doppler broadened lines used for ion temperature measurements in lower density plasmas.

5. Stark broadening

Critical data compilations of relevant parameters should be initiated as soon as a significant body of data becomes available.

REPORT OF THE WORKING GROUP ON PLASMA-SURFACE INTERACTION FOR FUSION NEEDS

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Introduction

The importance of plasma-surface interaction processes has increased since the IAEA Advisory Group Meeting in 1976 in Culham. With the advent of high-power beam heating experiments, and high power density, long-pulse reactor designs (such as INTOR) impurity effects are even more crucial.

Moreover, there has been a great expansion in the number of working experiments. There is a large number of specific materials presently used for walls, limiter and divertor plates; the number of materials which should be considered is thereby determined. Even more importantly it is now understood that the surface structure (especially topography and contamination) plays a determining role in most of the plasma-surface interactions. Hence, investigation of these processes must account for this basic fact if they are to have any relevance to fusion needs.

We consider basic plasma surface interactions for which data are needed, describe the materials of interest and the needed characterization of surfaces, and then present our recommendations for needed activities.

A. Particle-surface interactions

In this area we have revised and updated the report of the Surface Interactions Working Group of the 1976 Culham meeting, using this report as a guide. We have added some processes to the list to reflect recent advances, changed the relevant parameter range where necessary, and suggested a lower priority for some processes whose importance is felt to be diminished.

Several shorthand conventions will be used. In the tables below H* and He* means all isotopes and charge states of H and He correspondingly; surface structure* includes topography and contamination.

A.1 Reflection of H* (atoms and molecules) and He*

Primary energy:	Thermal to 10 keV.
Data to be measured:	reflection coefficient, energy and angular distributions (correlation with incidence angle), species, charge and excitation state.
Important parameters:	Angle of incidence, surface structure*.

A.2 Accommodation

a) H* (atoms and molecules) on wall and limiter materials (e.g. stainless steel, Inconel, graphite).

Primary energy:	0.01 eV to 1 eV.
Data to be measured:	accommodation coefficient.
Important parameters:	surface temperature, surface structure*.

b) Na and Cs on ion source materials (W, Ta, Mo, Rh, Pt, Au, Ag)

Primary energy:	0.04 eV to 1 eV.
Data to be measured:	accommodation coefficient.
Important parameters:	surface temperature, surface structure*.

A.3 Trapping of H* and He*

Primary energy:	100 eV to 400 keV for H*, up to 3.52 MeV for He*.
Data to be measured:	trapping coefficient.
Important parameters:	angle of incidence, temperature, dose, influence of radiation damage, surface structure* (most important).

A.4 Detrapping processes for H^* and He^*

Primary energy: 100 eV to 400 keV.

Data to be measured: time resolved release rate for thermal and beam-induced desorption of trapped gas.

Important parameters: angle of incidence, target temperature, influence of radiation damage, surface structure*.

A.5 Recombination of H^* (atoms and molecules) on surfaces

Primary energy: 0.1 eV to 200 eV

Data to be measured: rate of recombination, surface coverage.

Important parameters: surface temperature, surface structure*.

A.6 Sputtering by H^*, He^* and impurities

Primary energy: threshold to 400 keV.

Data to be measured: total yields, angular and, for particles emitted above 10 eV, energy distribution of sputtered materials; change in surface structure*.

Important parameters: angle of incidence, temperature (for multi-component surfaces), surface structure*.

A.7 Desorption by ions (H^*, He^*, and impurities) and electrons

Primary energy: threshold to 10 keV.

Data to be measured: cross-section, charge and excitation state, energy distribution.

Important parameters: angle of incidence, surface structure*.

A.8. Chemical reactions of H^* (atomic and molecular) ions

a) Erosion and impurity release

Primary energy:	thermal to 1 keV.
Data to be measured:	time resolved total yields and reaction products; excitation levels.
Important parameters:	surface temperature, surface structure*, flux density ($\leqslant 10^{18}/cm^2/s$) of incident particles.

b) Surface chemistry of molecular ions

Primary energy:	thermal.
Data to be measured:	time-resolved reaction products and changes in surface structure*.
Important parameters:	temperature, surface structure*.

A.9 Gettering

Primary energy:	thermal to 400 keV.
Data to be measured:	H retention.
Important parameters:	surface temperature, surface structure*, incident particles flux ($\leqslant 10^{18}/cm^2/s$).

A.10 Secondary electron emission due to ions and electrons

Primary energy:	threshold to 10 keV.
Data to be measured:	emission coefficients.
Important parameters:	surface structure*, angle of incidence.

A.11 Arcing

Quantitative estimates from calculation and experiment of time-resolved impurity production are needed (see recommendations).

A.12 Thermal shock: evaporation, mechanical response and integrity of composition

Input parameters: heat fluxes up to 5 kW/cm^2, rise time 20 ms.

Data to be measured: time-resolved release rate, changes in surface structure*.

Important parameters: composition (i.e. coating, cladding), surface structure*, predominant topography.

A.13 Other processes

a) Blistering: synergistic effects for energetic (up to 3.52 MeV) alpha particles.

b) Desorption by photons: efficiency of stimulated photo electron desorption (note remarks on surface structure in the introduction).

B. Surface materials of interest

The data needs for existing devices and projects determine the specific materials which we consider. The materials are often separated according to the atomic number Z (high, medium, low) of their constituants. Progress in recent years requires that we now consider cladding as well as the categories described in the 1976 Culham Advisory Group report. Other than for minor changes, this list is the same as that given in the IAEA-199 Report.

B.1 Alloys

These are of particular interest as being the constructional materials of present generation and the next generation machines. The most commonly used alloys are various types of stainless steel and Inconel.

B.2 Refractory materials, e.g. Mo, Nb, V, W and alloys

These are used in some present machines as limiters and may possibly be used in high temperature industrial reactors. However, the high atomic number (particularly of tungsten) and high cost of these materials constitute serious disadvantages.

B.3 Low and medium Z materials, e.g. C, SiC, B_4C, Al, Be, BeO, BN, Ti, TiC, TiB_2

These materials may reduce the total radiation because of their moderate atomic number and some have been used in tokamaks already with encouraging results. However, chemical effects leading to impurities are still unclear and temperature effects should be further evaluated in some cases, e.g. carbon.

B.4 Trapping materials

In applications where large fluxes of ions have to be pumped, e.g. in divertors, metals which react chemically with hydrogen are being used. Examples are Ti, Zr, Al-Zr alloy.

B.5 Coatings and claddings

This heading covers the use of materials on top of structural materials. These may either be coatings of the materials mentioned above, e.g. low and medium Z materials, or of thin metal foils. Films are also of interest because in practical devices those films are produced in the course of operation due to evaporation, sputtering, etc.

C. Characterization of surface

To produce data relevant to fusion, it is now understood that surface structure (i.e. topography and contamination) must first be specified.

The great variety of possible materials for consideration must be restricted to those used in present experiments and in specific projected designs (e.g. INTOR). Without this limitation, the formulation of data needs and the evaluation and compilation of data would be an impossibly large task.

Progress has been made in the development of discharge cleaning techniques, so that there is no need to conduct fusion experiments with significant uncontrolled low Z impurity contamination. Moreover, a degree of control over the surface structure has thereby been achieved.

Greater emphasis must be given to control the surface structure*. Especially for angular distributions of sputtered and reflected particles, the specific surface structure* is of special importance. In the case of multi-component alloys, where preferential sputtering can take place, the surface topography and composition is crucial.

D. Recommendations

D.1 Restriction of materials

In order to enhance the relevance of these studies to fusion, and so that smaller research groups can participate in IAEA's cooperative research program, we recommend that a restricted number of complex surfaces of interest to fusion be identified. This evaluation should be carried out by fusion experts, under the auspices of IAEA.

a) The experts should:

1. Settle upon a small number of materials for the study of the processes described in Section A. These materials should be those used in present devices or in specific planned projects.

2. Prescribe the surface structure (i.e. composition) for these materials.

b) Data compilation and evaluation activities should be concentrated on the small number of complex surfaces of interest to fusion which have been selected in this way.

D.2 Arcing

Arcing is less understood than most of the other processes described in Section A. Characterization of the plasma properties, although very uncertain, plays a decisive role. We recommend that an Advisory Group meeting be convened by IAEA with the following aims:

a) Characterize more completely the plasma properties near the wall during periods of instability.

b) Propose an experimental and theoretical program to improve quantitative estimates of impurity release during arcing.