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IAEA SPECIALISTS' MEETING ON

"ATOMIC AND MOLECULAR DATA FOR PLASMA EDGE STUDIES"

Vienna, 8-10 July 1987

Summary Report

Edited by

J.J. Smith

December 1987

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

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Abstract

Proceedings of the IAEA Specialists' Meeting on atomic and molecular data for plasma edge studies, convened by the IAEA Nuclear Data Section on 8-10 July 1987, at the IAEA headquarters in Vienna, Austria are provided.

Reviews of both the role and importance of atomic and molecular processes in the modelling and diagnostic analysis of the plasma edge and the status of the atomic and molecular collision and structure and spectra data bases were undertaken. The results of these analyses are provided in the reports of the working groups convened. Specific recommendations were made to inform the plasma physics and atomic and molecular physics communities of the importance, existence and needs of atomic and molecular data for plasma edge studies.

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I. Summary of the Meeting

Introduction

A Specialists' Meeting on Atomic and Molecular (A+M) Data for Plasma Edge Studies was convened by the IAEA Nuclear Data Section on 8-10 July 1987 at the IAEA headquarters in Vienna on the recommendation of the A+M Data Centre Network at its Sixth Meeting on 10-12 September 1986. The purpose of the Meeting was to identify the fundamental processes of importance in the plasma edge region of current and future envisaged fusion devices at conditions relevant to the plasma boundary or edge. Fourteen experts from eight member states attended the meeting, representing the most active research groups in both the A+M and plasma physics fields. A full list of participants is contained in Appendix I. The impact of A+M processes on edge plasma behaviour was considered and the data status of the collision processes taking place in the plasma edge and the data for the structure and spectra of edge plasma constituents were reviewed.

J.J. Smith was Scientific Secretary of the meeting. The meeting was chaired by Dr. M.F.A. Harrison for the first two days, while for the final day Dr. R.K. Janev acted as chairman. The meeting was opened by Dr. J.J. Schmidt, head of the IAEA Nuclear Data Section.

Meeting Proceedings

The adopted agenda is provided in Appendix II. The work of the meeting was split into two distinct parts. Firstly, presentations and reviews of the plasma physics needs and the status of the A+M data bases were made. On the completion of the individual presentations, three working groups were formed to provide detailed assessments of the data needs and present availability. The reports of the working groups are provided in full in this report. For copies of papers presented in the first session of the meeting, the author identified should be contacted, however, for information a brief description of each presentation is provided.

Dr. M.F.A. Harrison gave a comprehensive review of the data requirements for plasma edge studies. Dr. D.B. Heifetz discussed the role of atomic physics of H and He in edge plasmas. The inclusion of A+M processes in the DEGAS 3-D code for neutral transport modelling was described along with the application of atomic and molecular data in radiative power loss studies and analysis of divertor operation. Comments were also provided on the means of interfacing the data with modelling codes.

Dr. T. Kawamura provided an outline of modelling studies of the scrape-off layer produced by a simple solid limiter in a torodal system. In addition, several comments on atomic and molecular data needed for reliable modelling of a scrape-off layer, which has an important role in controlling the plasma-wall interaction and the performance of the main plasma confinement, were given.

Dr. M.A. Lennon presented a review of a compilation and assessment of the experimental and theoretical data on the electron impact ionisation of diatomic molecules, H_2, D_2, T_2, O_2, N_2, NO, CO, and polyatomic molecules, H_2O, D_2O, NH_3, ND_3, N_2O, NO_2, CO_2, CH_4, CD_2, CD_3, CD_4, C_2H_2, C_2H_4, O_3 from threshold to 500 eV. Processes studied include total ionisation, single ionisation, double ionisation and dissociative ionisation. For each reaction, a recommended cross section was given, based on a careful assessment of the available data. A bibliography of references for the compiled data was provided together with a graph for each process. Ionisation energies and appearance potentials for each molecular species, with reference sources were also tabulated.

Dr. R.K. Janev commented on collision processes involving excited species in fusion edge plasmas. Because of the larger cross sections for charge transfer, ionization, excitation and other processes it was emphasised that it is necessary to account for collisions from excited states, especially when there could be a significant metastable content in the edge plasma. It was also stressed that the complete range of vibrational, translational and rotational transitions should be considered.

Dr. V.A. Belyaev contributed a paper on recommended cross-sections and rates for electron inelastic collisions with helium atoms. Consideration was given to the use of specific experimental or theoretical data to arrive at recommended values while for other processes empirical formulae have been employed.

Atomic data for hydrogens in collisions with electrons, with relevance to boundary plasmas was reviewed by Dr. H. Tawara. The material presented has been subsequently published as an addenda to the Nagoya report IPPJ-AM-46, published in 1986, as Nagoya report IPPJ-AM-55.

The status of the atomic and molecular structure and spectra data bases was provided by Dr. W.L. Wiese. Detailed lists of references were assembled for wavelengths, energy levels, ionization energies and transition probabilities and lifetimes. It was expressed that the transition probabilities, for species excluding H(D,T) and He may not be available to sufficient accuracy and the knowledge of the data for molecules containg impurities may be limited.

Dr. R.A. Phaneuf reported on heavy particle collisions in the plasma edge. Available cross-section data for heavy-particle collision processes which play important roles in the edge plasma of magnetically-confined fusion devices were surveyed and reviewed. The species considered include H, H_2, He, C, O, Fe, and their ions. The most important heavy-particle collision processes occurring in the edge plasma are charge-exchange reactions. Excitation and dissociation processes were also considered. Emphasis is given to relative collision velocities corresponding to plasma ion temperatures in the 1-200 eV range. Evaluated or recommended data were presented where possible along with their estimated uncertainties, and gaps in the data base were indicated.

Report of the Working Group on Atomic and Molecular Data Requirements for the Edge Plasma

P. Bogen, H.W. Drawin, M.F.A. Harrison (Chairman),
D. Heifetz, T. Kawamura and P. Lee

Atomic and molecular data requirements for the edge plasma differ somewhat from those for the hotter core plasma. In particular, the edge region contains molecules and low energy atoms that arise from plasma - surface interactions and also from gas or pellet fuelling. Apart from conditions in the ablation cloud around a pellet, the energy of molecules tends to correspond to the wall temperature. The lowest energy of atoms tends to be the Frank Condon energy of dissociation whereas the upper limit of energy corresponds to the daughter products of change exchange with the plasma ions. (The relatively low rates of collisions with high energy injected atoms and with escaping high energy ions are not considered in this report). A further difference from the core plasma arises because of the combined effects of the relatively low temperature of the plasma edge and the relatively short residence time of ions in this region. Consequently there tends, (a) to be a preponderance of low charge state ions and (b) ions of medium and high Z elements do not become fully stripped. Plasma conditions relevant to the edge region range from $n \sim 10^{15}/cm^3$ and $T \sim 10eV$ in the high recycling zone of a reactor divertor to $n \sim 10^{12}/cm^3$ and $T \sim 500eV$ in the plasma edge of experimental discharges.

The elements (and isotopes) of greatest interest are:

H, D and T (atoms and molecules).

He (helium is a product of D/T fusion reactions; it is also used for diagnostic purposes and sometimes discharges are run in pure helium).

C, Fe Ni, Cr (carbon, stainless steel and nickel based alloys are the most common boundary materials in present day experiments; they also have reactor applications).

O (atoms and moleules; this element is a common impurity because of its high chemical activity).

Ne, Ar (These are used for diagnostic purposes. They may be used for enhancing radiation losses from the edge plasma of reactors).

The most important impurity molecules are:

CH_4 (methane and its dissociation products arise from [C+H] interactions at surfaces).

CO (which arises from [C+O] interactions at surfaces).

This list covers those species most likely to be encountered in present day experiments and envisaged reactors. It must inevitably change from time to time due to the application of new diagnostic techniques and/or the adoption of new boundary materials. A transitory, but immediate, example is the inclusion of copper in the divertor of ASDEX.

In the edge plasma, the significance of neutral particles (atoms and molecules) tends to decrease with distance from the boundary surface. In the case of ions, the charge state tends to increase with increase in the distance to the surface measured along the open magnetic field lines. Hydrogen molecules and low charge state impurity ions are of particular significance in high recycling divertors whereas, at limiters and at the vessel wall, plasma conditions are strongly sensitive to hydrogen change exchange and to ionisation of hydrogen molecules. Collisions occur most frequently with electrons because of their higher velocity, the exception being those heavy particle collisions, e.g. resonant charge exchange, whose very large cross sections outweigh their relatively low collision velocity. Atomic and molecular data are required in order to determine ionisation rates, radiation rates, dissociation rates and change exchange rates. Due to the inhomogeneous nature of the density, temperature and drift velocity of the plasma it is also necessary to know the velocity and spatial distribution of the neutral products after a collision. It is also necessary to know the energy of charged products but, because of the combined action of the confining magnetic field and of Coulomb collisions, the direction of charged products is of less importance. Elastic collisions between ions and neutrals may, in certain circumstances, be significant. A guide to plasma conditions and to the concentration of impurity species is presented in Table 1.

There are two broad classes of data applications. Firstly, there is plasma modelling used for interpretation of experimental results and for prediction of edge conditions in future devices such as reactors, and secondly there are the needs of particular diagnostic devices. These requirements differ in the sense that diagnostics tend to rely upon a specific atomic process, e.g. the emission of a particular spectral line, whereas modelling needs more global information, e.g. the total radiated energy associated with the dissociation of a molecule. Both types of data should be produced. The desirable accuracy for both atomic and molecular data used in modelling and diagnostics is about 20%.

Regarding priorities for data requirements; in the case of atomic species there is already a considerable amount of data for electron impact ionisation and for charge exchange but there is a sparcity of data relevant to determing radiation losses from impurities. Molecular interactions have only recently begun to receive the attention that they warrant in the edge plasma. Serious problems which face the fusion plasma modeller are (a) the diversity and magnitude of data sources and (b) the absence of global data in which several processes have been grouped together in order to produce simpler parameters which can be accommodated into plasma codes. The selection of data priorities in this report reflects this latter problem.

The following data requirements have been selected because (a) they are urgently needed for both experimental and theoretical understanding of the edge plasma and (b) much of the data exists but not in the form requested.

(1) The effective number of protons produced for the emission of a single photon in the case of the commonly observed lines of atomic hydrogen, e.g. H_α, H_β etc. This analysis must include those contributions which arise from hydrogen molecules and also include multi-step processes.

(2) The average amount of energy dissipated by electrons (and the fraction of this energy which is radiated) in order to produce H^+ and H by dissociation of hydrogen molecules H_2 and H_2^+.

(3) The average amount of energy dissipated by electrons and the fraction that is radiated in the production of He^+ from He.

(4) The number of photons emitted per ion produced (in collisional radiative conditions) for some of the characteristic lines of Li, O and C.

(5) Information regarding excitation of atoms and molecules leaving surfaces exposed to fluxes of electrons and ions.

Some of the data required for these global parameters are not directly available but it is important that informed estimates be made in order that the parameters can be derived.

Species	Plasma	
	Density [cm^{-3}]	Temperature [eV]
H^+, D^+, T^+	10^{12} - 10^{15}	5 - 500
	Edge plasma	
	Concentration [%]	
H, D, T	≦ 50	2 - 500
H_2, D_2, T_2	≦ 50	$(0.1)^*$ - < 10
He, He^+, He^{2+}	≦ 10	10 - 500
	Pure helium discharge →	10 - 500
Li^d	≦ 30	10 - 500
$Be^{d,l}$	≦ 10	10 - 500
$C^{d,l}$	≦ 10	10 - 500
O^i	≦ 5	10 - 500
Ne^i	≦ 2	10 - 500
Al^d	≦ 2	10 - 500
Si^i	≦ 2	10 - 500
Ar^i	≦ 2	10 - 500
Ti^i	≦ 2	10 - 500
Cr^i	≦ 2	10 - 500
Fe^i	≦ 2	10 - 500
Ni^i	≦ 2	10 - 500
Cu^d	≦ 2	10 - 500
$Mo^{d,i}$	≦ 0.1	10 - 500
$W^{d,i}$	≦ 0.1	10 - 500
CH_n (n=1 to 4)	≦ 10	$(0.1)^*$ - < 10
CO	≦ 10	$(0.1)^*$ - < 10

(*) Energy of molecule.
(d) Divertor target, average charge states ~ <2 to 3>.
(l) Limiter, charge states higher than for divertor.
(i) Impurity, for elements with Z > 10, maximum charge state ~ 10.

Table 1 - A Guide to Edge Plasma Conditions and Impurity Content.

Report of the Working Group on Electron Collision Data, Spectroscopic Data and Their Present Status

M.A. Lennon, J.J. Smith, H. Tawara (Chairman) and W.L. Wiese

1. Introduction

We have compiled a list of the most relevant species of molecules and atoms for the plasma edge region and briefly describe the availability and reliability of data for them, and we also point out the needs for specific data in the future.

It appears that generally, data involving atomic species and especially atomic spectroscopy data are more prevalent and of better quality than data involving molecules. Molecular species which might be present in the edge plasma region are not yet well specified and their production mechanisms are not well understood.

2. Molecules

In electron-molecule collisions, the following processes should play a role:

a) excitation
b) ionization (pure ionization and dissociative ionization)
c) dissociation
d) recombination.

In Table 1, we show the present status of availability and reliability of data for molecular species with accuracies labelled as follows:

A: data with uncertainties of ±25%
B: data with uncertainties of ±50%
C: data with uncertainties of a factor of two
D: data are available but with unknown accuracy.

General Comments

i) Processes are investigated and data are well documented only for H_2 (Note that the isotope effect should not be significant).

ii) Total net ionization cross section for other molecular species should also be reliable but partial ionization cross sections often show large discrepancies in shape and magnitude and are not considered to be reliable.

iii) Practically no reliable dissociation data exist except for H_2 and for some hydrocarbons.

iv) Some excitation data are available but their reliability is low except for H_2.

v) The velocity distributions of the dissociated atom and ion species are not well investigated except for H_2 and a few molecules.

3. Atoms and Moderately Charged Ions

The atomic species originate either from sputtering (mainly metallic) or dissociation / dissociative ionization or from injection for diagnostic purposes. Here excitation and ionization processes should be taken into account. In Table 2, we show the present status of electron collision data for atomic species of interest for plasma edge studies.

General Comments

i) Ionization cross sections are well known with good accuracies for low Z species and singly charged metallic ions. However, no reliable ionization cross sections for neutral metallic species, in particular those at low energies, are available, though some theoretical calculations are available for high energies.

ii) Excitation data are very scarce for heavy metallic species.

4. Spectroscopy of Atoms, Moderately Charged Ions and Molecules

The spectroscopic quantities of main interest are the wavelengths of spectral lines and their classifications, as well as atomic energy levels and atomic transition probabilities. In Table 3, we show the present status of data availability and quality. The letters have the same meeting as in Table 1.

5. Recommended References

i) Recommended data for electron impact excitation of atoms and ions

1) Recommended data on excitation of carbon and oxygen ions by electron impact (Collisions of carbon and oxygen ions with electrons, H, H_2 and He, ORNL-6090/V5. R.A. Phaneuf, R.K. Janev and M.S. Pindzola, editors).

2) Recommended data on atomic collision processes involving iron and its ions (to be published in Nuclear Fusion (1987)). A.E. Kingston and M.A. Lennon.

3) Report on recommended data, Atomic Data Workshop, Daresbury, 1985. K. Aggarwal, K. Berrington, K. Eissner and A. Kingston.

4) An evaluated compilation of data for electron impact excitation of atomic ions. JILA Data Center Report 30 (1985). J.W. Gallagher and A.-K. Pradhan.

ii) Recommended references of electron impact ionization of atoms and ions

1) Recommended data on the electron impact ionization of light atoms and ions. J. Phys. Chem. Ref. Data 12,891-916 (1983), K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith, [H-O].

2) Recommended cross sections and rates for electron ionization of atoms and ions: fluorine to nickel, UKAEA Report CLM-R270 (1986), M.A. Lennon,

K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray and F.J. Smith, [F-Ni]. This also contains the revised recommendations for H - O (to be published in J. Phys. Chem. Ref. Data, 1987).

3) Recommended cross sections and rates for electron ionization of atoms and ions for high Z species: Cu - U (to be published in 1988), M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray and F.J. Smith, [Cu-U].

4) Total and partial ionization cross sections for atoms and ions by electron impact. At. Data and Nucl. Data Tables 36, 167-353 (1987). H. Tawara and T. Kato, [H-U including H_2, N_2 and O_2].

iii) Recommended references for electron impact ionization and excitation of molecules

1) Electron excitation, dissociation and ionization of H_2, D_2, T_2, simple hydrocarbons and their ions. Phys. Scripta 23, 170-178 (1981), F.J. de Heer.

2) Atomic and molecular processes in hydrogen-helium plasmas. Princeton Plasma Physics Laboratory PPPL-TM-368 (1985), R.K. Janev, W.D. Langer, K. Evans and D.E. Post [to be published in Springer-Verlag, series on Atoms and Plasmas, Vol. IV (1987)].

3) "Electron impact ionization" T.D. Mark and G.H. Dunn (Editors), Springer Verlag, New York (1985).

4) Critical survey of electron impact ionization data for selected molecules (Preliminary report). Queen's University of Belfast, M.A. Lennon, D.S. Elliott and A. Crowe (to be published as a Culham report).

5) "Electron-molecule interaction and their applications" Vol. 1, L.G. Christophrou, Academic Press, London (1984).

6) Electron scattering by molecules. II. Experimental methods and data. Phys. Rept. 97, 219-356 (1983), S. Trajmar, D.E. Register and A. Chutjian.

7) Atomic data involving hydrogens relevant to edge plasmas. IPPJ-AM-46 (Inst. Plasma Phys., Nagoya University 1986), H. Tawara, Y. Itikawa, Y. Itoh, T. Kato, H. Nishimura, S. Ohtani, H. Takagi, K. Takayanagi and M. Yoshino.

8) Atomic collision processes in plasma physics experiments. UKAEA Report CLR-R137 (1974), R.L. Freeman and E.M. Jones.

iv) Recommended spectroscopic data tables

A) Atoms and ions

a) Wavelengths

1) "Wavelengths and transition probabilities for atoms and atomic ions". NSRDS-NBS 68. U.S. Government Printing Office, Washington, D.C. (1980), J. Reader, C.H. Corliss, W.L. Wiese and G.A. Martin (contains 47000 lines of neutral atoms and the first four stages of ionization).

2) "Selected tables of atomic spectra". NSRDS-NBS 3, U.S. Government Printing Office, Washington, D.C., C.E. Moore. (Sections 1 - 3 (1965, 1967, 1970); 6(1972); 7(1976); 8(1979); 9(1980); 10(1982); 11(1985): tables for H I, D I, C I-VI, O I-VIII, Si I-IV).

3) Tables of vacuum ultra-violet lines. J. Phys. Chem. Ref. Data, Supplement (to be published in 1987), R. Kelly.

b) Atomic energy levels

1) "Selected tables of atomic spectra", NSRDS-NBS 3, U.S. Government Printing Office, Washington, D.C., C.E. Moore (Section 3(1970); 6(1972); 7(1976); 8(1979); 9(1980); 10(1982); 11(1985) (energy levels for H I, D I, C I-VI, O I-VIII).

2) Energy levels of neutral helium. J. Phys. Chem. Ref. Data 2, 257 (1973), W.C. Martin.

3) Energy levels of aluminum: Al I through Al XIII. J. Phys. Chem. Ref. Data 8, 817 (1979), W.C. Martin and R. Zalubas.

4) Energy levels of silicon, Si I through Si XIV. J. Phys. Chem. Ref. Data 12, 323 (1980), W.C. Martin and R. Zalubas.

5) Atomic energy levels of the iron period elements: potassium through nickel. J. Phys. Chem. Ref. Data 14, Supplement No. 2 (1985), J. Sugar and C. Corliss (contains the energy level data for K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co and Ni).

6) Energy levels of molybdenum, Mo I through Mo XLII. J. Phys. Chem. Ref. Data (to be published in 1987), J. Sugar.

7) "Atomic energy levels", NSRDS-NBS 35, Vol. I-III, U.S. Government Printing Office, Washington, D.C. (1971). (contains data for all elements not listed above).

c) Ionization potentials

"Ionization potentials derived from the analysis of optical spectra". NSRDS-NBS 34, U.S. Government Printing Office, Washington, D.C. (1970), C.E. Moore.

d) Atomic transition probabilities

1) "Atomic transition probabilities, Vol. I, hydrogen through neon", NSRDS-NBS 4, U.S. Government Printing Office, Washington, D.C. (1966), W.L. Wiese, M.W. Smith [H, He, Li, Be, B, C, N, O, F, Ne].

2) "Atomic transition probabilities, Vol. II, sodium through calcium". NSRDS-NBS 22, U.S. Government Printing Office, Washington, D.C. (1969), W.L. Wiese, M.W. Smith and B.M. Miles [Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca].

3) Atomic transition probabilities, Scandium through nickel, J. Phys. Ref. Data, Supplement (to be published in 1988), G.A. Martin, J.P. Fuhr, W.L. Wiese and A.W. Weiss. [Sc, Ti, V, Cr, Mn, Fe, Co, Ni].

4) (See ref. iv.A.a.1) for transition probabilities of heavy elements.

e) Comprehensive spectroscopic compilation for specific elements

1) "Spectroscopic data for iron" ORNL-6089. W.L. Wiese and A. Masgrove (to be published in 1988).

2) "Spectroscopic data for Ti, Cr and Ni" ORNL-6089. W.L. Wiese and A. Robey (Editors) (to be published in 1988).

B) Molecules (H_2, HD, D_2)

1) "Wavelength tables of the H_2 spectrum from 2800-2900 Å, with assignments for many lines", H. Crosswhite (John-Wiley Int. (1972)).

2) Tables of energy levels for H_2, J. Mol. Spectr. 2, 494 (1958), G.H. Dieke.

3) Potential energy curves for H_2, At. Data 2, 119 (1971), T.D. Sharp.

4) "Molecular spectra and molecular structure" Vol. IV, constants of diatomic molecules, (van Nostrand-Reinhold Pub.), G. Herzberg (contains detailed spectral data on H_2, HD and D_2).

6. Recommendations to the Atomic and Molecular Physics Community for Future Work

Based upon the present survey, it appears important that the following for electron impact collisions and spectroscopic data should be determined:

i) Cross sections for the dissociative ionization and simple dissociation of molecules.

ii) Cross sections for the velocity distribution (and angular distribution) of dissociated atoms and ions.

iii) Cross sections for the excitation of molecules.

iv) Cross sections for the ionization of neutral heavy metallic species.

v) Cross sections for the excitation of neutral atoms and ions with low charges (both low and high Z).

vi) Transition probabilities for heavy metals (and molecules).

Table 1: Electron collisions with molecules and molecular ions

Species	Excitation	Ionization Total	Ionization Partial	Dissociation	Dissociative Recombination
H_2	A	A	B	A	C
CH_4	D	A	B	D	
CH_3			B		
CH_2			B		
CH					
C_2H_2	D	A		D	
C_2H_4	D	A	B		
H_2O	D	A	C	D	
C_2					
CO	D	A	C	D	
CO_2	D	A	C	D	
O_2	D	A	C	D	
H_2^+	D		B	B	B
H_3^+			B	B	B
CO_2^+			B		
H_2O^+					
CH_4^+					

Table 2: Electron collisions with atoms and ions

Species	Excitation	Ionization neutral	Ionization singly charged
H	A	A	–
He	D	A	A
Li	D	A	A
Be	D	A	A
C	A	A	A
O	A	A	A
Ne	D	A	A
Al	D	B	A
Si	D		A
Ar	D	A	A
Ti	D	B	A
Cr	D	C	A
Fe	A	C	A
Ni	D	C	C
Ga	D		A
Kr	D	A	A
Mo	D	C	A
Xe	D	A	A
Zr	D	C	
Ta	D		
W	D		A

Table 3: Spectral data

Atoms and moderately charged ions

Species	Wavelengths	Energy levels	Trans. Prob.
H(D,T)	A	A	A
He	A	A	A
Li,Be,C,O	A	A	B
Ne,Al,Si,Ar	A	A	B
Ti,Cr,Fe,Ni	A	A	C
Zr,Mo,Ta,W	B	B	(C)*

* Only few data are available.

Molecules

H_2,HD,D_2	A	A	B
others	A-B	A-B	C

Report of the Working Group on Heavy-Particle Collisions in the Edge Plasma

F. Aumayr, R.K. Janev and R.A. Phaneuf (Chairman)

Abstract

A summary is presented of the role of inelastic collisions between heavy particles in the edge region of magnetically confined fusion plasmas. An assessment is given of the relative importance of the various processes occurring in the plasma edge, and of the status of the relevant atomic data base.

1. Introduction

The key role of atomic and molecular collision processes in the edge region of magnetically confined plasmas has been addressed during the last few years in several articles [1-3]. Of particular significance is a recent compilation of edge-plasma relevant atomic-collision data involving hydrogen atoms, molecules and ions by Tawara and co-workers [4]. A number of other data compilations also contain information on specific collision processes between heavy particles which occur in the plasma edge region [5-14].

Because heavy particles are considerably more massive than electrons, their velocity at the same plasma temperature is significantly lower (by a factor of $(1836 \times A)^{1/2}$ for a heavy particle of mass A in amu). The collisional rate coefficient $<\sigma v>$ scales linearly with the relative particle velocity v. Therefore, in order to have a collisional rate which is comparable to that for electron collisions, the cross section for a given collision process between heavy particles must be substantially larger to compensate for the reduced frequency of collisions between heavy particles in the plasma.

The heavy-particle collision processes which are considered, in roughly their order of importance in the edge plasma are: charge exchange, vibrational excitation and dissociation of molecules, interchange reactions, electronic excitation, and ionization. Inelastic processes may be generally classified as to whether they are endoergic, resonant or exoergic. Endoergic processes have some well-defined threshold energy, usually of the order of a few eV to several tens of eV for the species present in the edge and the processes listed above. In general, cross sections for inelastic heavy-particle collisions tend to be largest at relative collision velocities which are close to the velocities of the active bound electrons in the system. For endoergic processes, the cross section decreases with decreasing energy, becoming exponentially small at the lowest energies. Resonant or exoergic processes, on the other hand, are characterized by cross sections which increase with decreasing energy, and these may play an important role at the low temperatures prevailing in the edge plasma.

Table I presents a summary of the heavy-particle processes considered for a number of reactants which might be expected to be present in the edge plasma, along with comments concerning the availability and reliability of the data, and the relative importance of that process in the edge. In general, the relative importance of a given process is determined by the total reaction rate, which is expressed as the product of the reaction rate coefficient times the concentrations of each reactant. Other factors such as competing processes or the effect of a particular process on the particle and energy balance, or on diagnostics have also been considered. Specific references to the most recent data compilations or other data sources are also given.

2. Charge-Exchange Reactions

Many charge-exchange (electron-capture) reactions proceed via crossings of potential-energy curves, and are either resonant or exoergic. Examples are symmetric charge-exchange reactions, which are exactly resonant, and charge exchange reactions involving multiply ionized plasma impurities. The latter are generally exoergic, populating excited levels of the product ion, and are important for radiative cooling of the edge as well as for diagnostics. Total cross-section data are available for most of the reactions considered, although not always at the lowest energies for a number of reactions between H, H_2 and He atoms and ions. He-like ionization stages will be strongly populated for C and O impurities in the edge, and heavier impurities such as

Fe and Ni will exist in ionization stages as high as 10-15. Recommended total cross-section data are available for most reactions involving partially-stripped C, O [11] and Fe [13] impurity ions colliding with H, H_2 and He. Partial cross sections for populating specific excited product states are also available for many of these reactions involving C^{q+} and O^{q+} ions [15-17]. Total cross sections for electron capture by other partially-stripped heavy impurities from H, H_2 and He may be estimated using established scaling rules, which have been shown to be reliable to 25% for charge states 5+ and above [13].

Electron-capture collisions of impurities with metastable H and He have in general larger cross sections than those for ground-state atoms and may be estimated from theoretical considerations [5]. Due to the Coulomb repulsion of the reactants, charge-exchange collisions between positive ions have very small cross sections at low energies [18, 19] and may be neglected for most edge-plasma modelling applications.

3. Vibrational Excitation of Molecules

Due to the fact that momentum transfer is more efficient for collisions between particles whose mass is comparable, the peak cross sections for vibrational excitation of molecules by proton impact are larger than those for electron impact. Such processes should therefore be considered in regions of the edge plasma where molecules are abundant. Such data are available for vibrational excitation in $H^+ + H_2$ collisions [4]. Electron-capture collisions involving vibrationally excited H_2 may also be enhanced. Vibrational-translational energy transfer is expected to play a role in the energy balance of the edge.

4. Interchange Reactions

Heavy-particle interchange in collisions of molecular ions with molecules may have very large cross sections at eV energies, and thus play a role in the edge plasma. Exchange reactions involving isotopes of hydrogen will be most important for tritium transport and inventory in ignited plasmas. Data are available for reactions of the type $H_2^+ + D_2 \rightarrow D_2H^+ + H$ and isotopic variations thereof [4].

5. Electronic Excitation, Ionization and Dissociation

These processes are all endothermic, having well-defined threshold energies. Almost no data are available for these reactions at the collision energies relevant to the plasma edge. However, the cross sections will be relatively small ($<10^{-18}$ cm^2) at these low energies, and thus electron-induced collisional excitation, ionization and dissociation will dominate by several orders of magnitude over the same processes induced by proton collisions, due to the increased frequency of electron collisions.

6. Summary

Among heavy-particle collisions at the temperatures and collision energies present in the edge plasma, charge-exchange is by far the dominant inelastic process. While compiled experimental and/or theoretical data are available for most of the important reactions, cross sections in a number of cases do not extend down to energies below a few keV/amu. Thus some extrapolation is required, producing a large uncertainty in some cases. Such is the situation for a number of charge exchange reactions among H, H_2, He, and their ions. With a few exceptions, the charge-exchange data base for C, O, and Fe impurities is reasonably complete and reliable. Scaling laws based on existing data and theoretical considerations may be applied to obtain estimates for other heavy impurity species in the plasma. Data for collisions of primary plasma constituent ions (e.g., H^+) with neutral metallic impurities are not generally available, except for Li, and little data are available for collisions involving excited species. Compiled data for vibrational excitation by proton impact are available for H_2, as well as for heavy-particle interchange reactions involving H_2 and isotopic derivatives.

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Table 1. Heavy-particle reactions in the edge plasma (energy range 1 eV - 200 eV)

Particle 1 (ion)	Particle 2 (atom/molecule)	Charge Exchange	Vibrational Excitation	Dissociative Excitation	Excitation, Ionization	Comments
H^+	H	A			U	
	H*	B			U	
	H_2, $H_2(v)$	A,ϕ	B	U	U	
	He	U			U	
	He*	B or C			U	
	C	U			U	
	O	A			U	
	M	ϕ			U	(M = Li, Be, Ti, Fe,
	CO	B	ϕ	ϕ	U	Cr, Ni, Ga, Al, V,
	CH_4	B	ϕ	ϕ	U	Nb, Mo, W)
H_2^+	H	B	ϕ	U	U	
	H*	ϕ	U	ϕ	U	
	H_2, $H_2(v)$	A,ϕ	ϕ	U	U	
	He	U	ϕ	U	U	
	He*	ϕ	ϕ	ϕ	U	
	C	ϕ	ϕ	ϕ	U	
	O	ϕ	ϕ	ϕ	U	
	M	ϕ	ϕ	ϕ	U	
	CO	ϕ	ϕ	ϕ	U	
	CH_4	ϕ	ϕ	ϕ	U	

Availability and accuracy:

ϕ - no data available.
A - accuracy better than ±20%.
B - accuracy better than ±50%.
C - accuracy better than ±100%.
U - unimportant process in edge plasma (rate < 10^{13} cm^{-3} s^{-1}).

Table 1 (Contd.)

Particle 1 (ion)	Particle 2 (atom/molecule)	Charge Exchange	Vibrational Excitation	Dissociative Excitation	Excitation, Ionization	Comments
He^{+}	H	U			U	
	H*	ϕ			U	
	H_2, $H_2(v)$	U,ϕ	ϕ	U	U	
	He	A			U	
	He*	ϕ			U	
	C	U			U	
	O	U			U	
	M	U[†]			U	[†]M = Li: ϕ
	CO	ϕ	ϕ	ϕ	U	
	CH_4	ϕ	ϕ	ϕ	U	
He^{2+}	H	B or C			U	Main capture process: $He^{2+}+H \rightarrow He^{+}(n=2)+H^{+}$
	H*	B[†]			ϕ	[†]Theory [5]
	H_2, $H_2(v)$	U,ϕ	ϕ	ϕ	U	
	He	A[§]			U	[§]Refers to double capture. Single capture is unimportant.
	He*	ϕ			U	
	C	U			U	
	O	ϕ[¶]			U	[¶]Capture into He(n=2)
	M	ϕ			U	
	CO	ϕ	ϕ	ϕ	U	
	CH_4	ϕ	ϕ	ϕ	U	

Availability and accuracy:

- ϕ – no data available.
- A – accuracy better than ±20%.
- B – accuracy better than ±50%.
- C – accuracy better than ±100%.
- U – unimportant process in edge plasma (rate $< 10^{13}$ cm^{-3} s^{-1}).

Table 1 (Contd.)

Particle 1 (ion)	Particle 2 (atom/molecule)	Charge Exchange	Vibrational Excitation	Dissociative Excitation	Excitation, Ionization	Comments
C^{q+}	H	A,B(q=1)			U	
	H*	ϕ			U	
q = 1 - 4	H_2,H_2(v)	A,ϕ	ϕ	ϕ	U	
	He	B†			U	†No data for C^+ + He
	He*	ϕ			U	
O^{q+}	H	A			U	
	H*	ϕ			U	
	H_2,H_2(v)	B,ϕ	ϕ	ϕ	U	
q = 1 - 6	He	B			U	
	He*	ϕ			U	
Fe^{q+}	H	A,B(q=1)			U	
	H*	ϕ			U	
	H_2,H_2(v)	A,B(q=1)	ϕ	ϕ	U	
q = 1 - 15	He	B,C(q<4)§			U	§Based on scaling formula
	He*	ϕ			U	
M^{q+}	H	C,B(q>5)			U	Based on scaling formulae
	H_2	C,B(q>5)			U	
	He	C,B(q>5)			U	

Availability and accuracy:

ϕ - no data available.
A - accuracy better than ±20%.
B - accuracy better than ±50%.
C - accuracy better than ±100%.
U - unimportant process in edge plasma (rate $< 10^{13}$ cm^{-3} s^{-1}).

Conclusions and Recommendations of the Meeting

(Prepared by R.K. Janev)

The Specialists' Meeting on Atomic and Molecular (A+M) Data for Plasma Edge Studies has discussed in depth the impact of atomic and molecular processes on edge plasma behaviour, its transport and radiation properties, hydrogen and impurity recycling, divertor physics, radiation cooling and other confinement relevant aspects. The edge plasma parameters and composition were defined on the basis of their values in the currently operating magnetic confinement devices, as well as those anticipated for the next step fusion test facilities. The data status of A+M collision processes taking place in fusion edge plasmas, and the data for the structure and spectra of edge plasma constituents, have been thoroughly analyzed, particularly from the point of view of modelling and diagnostics of these plasmas. It has been found that there exists a large amount of evaluated data for the basic collision processes between the major plasma constitutents. However, it has also been found that there are many gaps in the required data base, particularly for processes involving hydrogen molecules and ions, low charged metal impurity ions, and carbon-containing compounds ($C_k H_n$, CO, ...). The data base regarding structure and spectra of edge plasma constituents was found to be much more complete. All these findings are systematically presented in the preceding reports of the working groups.

In order to meet the data needs for edge plasma modelling and diagnostics in the current and future magnetic fusion experiments, the following has been concluded and recommended:

1. To make the fusion community aware of the existence of a large body of evaluated A+M data pertinent to edge plasma conditions, and to indicate the sources where these data can be found. It has been suggested that an information (Report from the Meeting) be published in "Nuclear Fusion". H. Drawin, M.F.A. Harrison and R.K. Janev were proposed to write this Report and submit it for publication by the end of 1987.

2. To make the atomic physics community aware of the A+M data needs for edge plasma studies and promote data production work in laboratories. It has been suggested that an information (Report) on this be published in "Comments in Atomic and Molecular Physics", which should shortly present the data status and indicate the data needs for specific collision processes. R.A. Phaneuf, H. Tawara and D. Heifetz were proposed to write this report and submit it for publication by the end of 1987.

3. In order to fill in the gaps in the A+M data base for edge plasma studies, it has been suggested that the IAEA A+M Data Unit organize a Coordinated Research Programme (CRP) on the Production and Evaluation of A+M Collision Data for the Plasma Edge, starting 1987. Parellel to the A+M data production work, a data evaluation work should be carried out in the Atomic Data Centres. The CRP should concentrate on the most urgently needed data and extend over a period of three years.

APPENDIX I

List of Participants

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APPENDIX II

Specialists' Meeting on Atomic and Molecular Data for Plasma Edge Studies

IAEA, Vienna, 8 - 10 July 1987

Adopted Programme

Wednesday, 8 July 1987

Morning Session: Chairman: Dr. M.F.A. Harrison

9.00 Opening of Meeting by Dr. J.J. Schmidt

9.30 Introduction and overview of the data requirements for Plasma Edge Studies.
- Dr. M.F.A. Harrison

10.30 Discussion

11.00 Coffee

11.30 Roles of the Atomic Physics of H and He in Edge Plasmas.
- Dr. D.B. Heifetz

12.30 Discussion

Afternoon Session: Chairman: Dr. M.F.A. Harrison

14.00 Comments on atomic and molecular data needed for scrape-off layer modelling.
- Dr. T. Kawamura

14.30 Discussion

14.45 Review of electron impact ionization data.
- Reviewer: Dr. M.A. Lennon

15.30 Discussion

16.00 Coffee

16.30 Collision processes involving excited species in fusion edge plasmas.
- Dr. R.K. Janev

Thursday, 9 July 1987

Morning Session: Chairman: Dr. M.F.A. Harrison

9.00 Recommended Cross-sections and Rates for Electron Collisions with Helium Atoms.
- Dr. V.A. Belyaev

9.30 Discussion

9.45 Atomic data for hydrogen in collisions with electrons - relevance to boundary plasmas.
- Reviewer: Prof. H. Tawara

10.45 Discussion

11.00 Coffee

11.30 Atomic radiation data for cool plasmas.
- Dr. W.L. Wiese

12.10 Discussion

12.15 Review of heavy-particle collisions in the plasma edge.
- Reviewer: R.A. Phanuef

12.45 Discussion

12.50 Formation of working groups to evaluate needs and availability of atomic and molecular data for the plasma edge. The following working groups were constructed:

- Study group for heavy particle collisions
- Study group for electron induced collisions
- Plasma physics for modelling and diagnostics group

Afternoon Session:

14.00 Meeting of working groups.

16.00 Preliminary reports of working groups.

Friday, 10 July 1987

Morning Session:

9.00 Meeting of working groups.

Afternoon Session: Chairman: Dr. R.K. Janev

14.00 Meeting of working groups.

15.00 Reports of the working groups.

16.00 Definition of follow up actions to be undertaken and conclusion of meeting.