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IAEA ADVISORY GROUP MEETING ON
"ATOMIC AND MOLECULAR DATA FOR FUSION PLASMA IMPURITIES"

Vienna, September 25-27, 1991

SUMMARY REPORT

Prepared by R.K. Janev

February 1992

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

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Abstract

This Summary Report briefly summarizes the proceedings, conclusions and recommendations of the IAEA Advisory Group Meeting on "Atomic and Molecular Data for Fusion Plasma Impurities", held at the IAEA Headquarters in Vienna on 25-27 September 1991. The reports of the two Meeting Working Groups regarding the data status and needs for spectroscopic and collisional data on plasma impurities are also included.

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1. INTRODUCTION

On recommendation by the Subcommittee on Atomic and Molecular (A+M) Data for Fusion of the International Fusion Research Council, given at its 6th Meeting (October 1990), the IAEA A+M Data Unit convened on September 25-27, 1991, an Advisory Group Meeting on "Atomic and Molecular Data for Fusion Plasma Impurities" at the IAEA Headquarters in Vienna.

The Meeting objectives were:

1) to assess the A+M data status and needs for the most important fusion plasma impurities, and
2) to prepare recommendations to the IAEA A+M Data Unit regarding its activity in this area.

One of the specific objectives of the Meeting was the prioritization of the tasks within the initiated IAEA Co-ordinated Research Project on "Atomic data for medium- and high-Z impurities in fusion plasmas", resulting from the recently formulated near- and long-term R+D plans related to the Engineering Design Activities (EDA) of International Thermonuclear Experimental Reactor (ITER). Impurity control is identified as one of the critical issues of the ITER engineering design and is becoming a dominant research subject in the current large tokamak experimental activities (JET, JT-60, Tore Supra) in support to ITER EDA. Accurate information on spectroscopic, radiative and collisional characteristics of fusion plasma impurities is required for modelling the radiative plasma power losses, impurity transport in the central and edge plasmas and for spectroscopic and active beam diagnostics of parameters of these plasmas. The information on radiative and collisional characteristics of impurities is also crucial for several fusion reactor design issues such as radiative cooling of the edge plasma, impurity shielding capability of the scrape-off layer, impurity recycling in the plasma edge, etc.

The Meeting addressed the following types of data for plasma impurities:

a) Spectroscopic data (energy levels, wavelengths, transition probabilities),
b) Electron-impact collisional data (excitation, ionization, recombination),
c) Data for impurity ion collisions with H, H_2 and He,
d) Data for radiative cooling rates of plasma impurities.

The Meeting was attended by 17 participants (see Appendix 1: List of Meeting Participants). During the preparatory stage of the Meeting, the participants prepared either overviews of the data situation for the above categories of data, or significant sets of new, original data for some classes of collision processes. The IAEA A+M Data Unit has also provided a background information on the work done at previous IAEA meetings on subjects within the scope of the present Meeting.

2. MEETING PROCEEDINGS

After the opening of the meeting and adoption of Meeting Agenda (see Appendix 2), the work of the meeting proceeded in the following sessions:

1) Spectroscopic and electron-impact collision data,
2) Data for heavy-particle collisions,
3) Data for heavy-particle collisions and plasma applications of atomic data,
4) A+M data status and needs for fusion plasma impurities,
5) Meeting conclusions and recommendations.

In this section we shall describe the highlights of the Meeting presentations and discussions. In the next section we shall reproduce the Working Group Reports, containing the results of the analysis for different types of data on plasma impurities and in Section 4 we give a summary of meeting conclusions and recommendations.

The session on spectroscopic and electron-impact collision data started with a comprehensive review by W.L. Wiese on the availability and quality of the energy level, wavelength and transition probability data for all fusion relevant plasma impurities. Dr. Wiese discussed deficiencies in the spectroscopic data bases, particularly for elements with $Z > 26$. A critical analysis of the recent data on atomic transition probabilities provided both experimentally and theoretically (particularly within the OPACITY project) was also presented, stressing the problems which appear in the process of accuracy assessment of these data. A.Ya. Faenov reviewed the content of spectroscopic data base for plasma impurities in the Centre for Highly Charged Ions at the VNIIFTRI (Mendeleevo). He also discussed the current data evaluation and data generation activity of that Centre, as well as their future plans. In a well balanced and in-depth presentation L.A. Vainshtein provided details on the structrue, physical basis and data generation capabilities of the numerical code ATOM developed at the P.N. Lebedev Physical Institute (Moscow). The code solves the single-electron radial Schrödinger equation for a selected "active" atomic electron with externally provided energies and uses the obtained wavefunctions for calculation of matrix elements involved in radiative transitions and electron-impact processes (excitation, ionization, radiative and dielectronic recombination, etc). For the needs of the Meeting, a number of excitation transitions in the He-, Li-, Be-, B- and Ne-like ions of Ni have been calculated by the ATOM code.

In the session on heavy-particle collisions, a significant number of new cross section results on electron capture and ionization processes have been reported by D.R. Schultz performed by using the Classical Trajectory Monte Carlo (CTMC) method. It was demonstrated that for the intermediate-Z impurities, the ionization and total electron capture cross sections do not reveal any Z-dependence (for a fixed ionic charge q), thus substantiating the q-scaling of the CTMC cross sections for these processes at least for $q \gtrsim Z/2$. Whether this feature of CTMC results persists also for the lower q-values is at present unclear and requires further elaboration both of the method itself and the representation of the effective electron-ionic core interaction. A large number of ionization electron capture (including shell selective) CTMC cross sections for collisions of incompletely stripped impurity ions with H and He have been presented by K. Katsonis. In the case of the He target (treated within the independent particle model) due attention in these calculations has been paid to the unitarity of the scattering process (i.e. two-electron transition processes have been explicitly taken into account). The ionization of hydrogen atoms (also in an excited state) by slow fully stripped ions was addressed in the talk by I.V. Komarov within the concept of promotion of the system to the continuum through series of hidden adiabatic energy crossings. A general formula was presented describing the contribution to the ionization cross section coming from the super-promotions at small internuclear distances (which are the dominant ones at very low collision velocities). Within the same adiabatic super-promotion model, P.S. Krstic reported excitation and ionization cross sections for the slow collisions of He^{2} with H(1s) and H(n=2). More than 120 molecular states were included in these calculations.

H. Tawara presented the electron capture data requirements for the design of an aparatus for measurement of electromagnetic fields in large tokamak plasmas. A detailed account of these data needs is given in Appendix 3. T. Shirai presented a brief summary of the data activities in the JAERI A+M Data Unit related to fusion plasma impurities. The presentation included activities in both spectroscopic and collision data areas.

A part of session 3 was devoted to the data base for radiative cooling rates of impurities in fusion plasmas. V.A. Abramov presented intercomparison of radiative cooling rates for Fe, Mo and W obtained by using different atomic data bases. It was shown that the sensitivity of cooling rates on atomic data used is high, especially for edge plasma temperatures (1-100 eV). R. Marchand presented extensive radiative and electron-energy loss calculations for the carbon and oxygen impurities in the plasma temperature range from 10 eV to 40 keV. The plasma model used in these calculations accounts explicitly for the presence of metastable species. The IAEA recommended atomic data bases were used in these calculations. Preliminary results for the radiative cooling rates for He and Fe impurities were also presented.

After a general discussion in Session 4 on the A+M data status and needs for plasma impurities, the work of the Meeting proceeded within two Working Groups (WGs): WG on spectroscopic and electron-impact collision data and WG on heavy-particle collision data. The tasks of these groups were to perform a detailed analysis of the completness and quality of existing data, to identify the most urgent data needs with respect to the current fusion research and reactor design programmes, and to make recommendations to the IAEA regarding the priorities in its activity in this area. The results of the working groups' discussions and analyses are given in their reports, reproduced in the next section. A particular set of atomic data needs related to the optimization of the neutral beam injection system for fusion reactors was discussed in the Working Group on heavy-particle collisions. These data needs, formulated in general terms by V.A. Belyaev, are outlined in Appendix 4.

In the last plenary session of the Meeting, the working group reports were discussed by all participants and several general conclusions and recommendations were made regarding the atomic data status and needs for plasma impurities. These are summarized in Section 4 of the present Report.

3. WORKING GROUP REPORTS

3.1. SPECTROSCOPIC AND ELECTRON-ION COLLISION DATA FOR PLASMA IMPURITIES

A. Faenov, R. Marchand, H. Tawara, L. Vainshtein, W. Wiese (Chairman)

A. Introduction

In this report we critically review and summarize the available spectroscopic and electron-ion collision data which are of primary importance to fusion research. We address plasma impurities on present and future fusion research machines and include also some elements, such as Li, Ne and Ar, which are not impurities per se, but are introduced for diagnostic purposes.

In a series of recent advisory meetings at the IAEA, various electron-ion collision data have been already reviewed for specific groups of plasma impurities, such as Helium[1], beryllium and boron[2], carbon and oxygen[3], and intermediate Z metallic elements[4] in the range $22<Z<29$. We therefore refer to these reports for details and shall not repeat the same information here. Instead, we turn our attention primarily to the heavy metal impurities Ga, Mo, Ta and W plus three light elements utilized (or considered) for diagnostics: Li, Ne and Ar.

B. Current Data Situation

1. Spectroscopy Data:

The spectroscopic data situation has not been discussed in the earlier cited IAEA advisory meetings, except for the C and O impurities.[3] We therefore review the status of spectroscopic data in toto. Extensive data are available for most of the chemical elements of fusion interest, including many pertinent ions. However, there is a noticeable degradation in quality and completeness from the lighter to the heavier elements, and for numerous ions of heavy elements almost no data are available as yet. The data are summarized in Table 1, where the the elements of interest are divided into three groups.

TABLE 1. STATUS OF SPECTROSCOPIC DATA

Elements, Including Ions	Completeness	Quality
1. H, He, Li, C, N, O, Be, Ne:		
Energy Levels	High	Excellent
Wavelengths	High	Excellent
Transition Probabilities	High	Often very good (<5%), but some only fair
2. Ar, Ti, Cr, Fe, Ni, Cu:		
Energy Levels	Moderate	Excellent
Wavelengths	Moderate	Excellent
Transition Probabilities	Some Large Gaps in Data	Fair (±10 to ±50%)
3. Mo, Ta, W		
Energy Levels	Poor (few data)	Very good
Wavelengths	" " "	" "
Transition Probabilities	" " "	Most data of poor quality (factors of 2), but Mo I in good shape

Completeness and quality of data are listed for (a) wavelengths and energy levels (these quantities are closely related) and (b) for transition probabilities. Energy level and wavelength data--especially the experimental data--are typically of very high accuracy, usually better than 1 part in 10^5 and often 1 part in 10^6. Transition probability data, which are by orders of magnitude less accurate than energy levels and wavelengths, are typically available with accuracies ranging from 5 to 20% for the light elements, in the range from 10 to 50% for medium heavy elements and are often much less accurate for complex heavy elements. A complete listing of all spectroscopic data tables compiled at the U. S. National Institute of Standards and Technology (NIST) is given in the IAEA Techn. Report INDC (NDS)-243/M7(1990).[5]

A comprehensive bibliographic database is being built up at NIST and contains at present about 25,000 literature references. Also, two comprehensive numerical databases of critically evaluated spectroscopy data are in operation at NIST and at VNIIFTRI, and are being updated and enlarged.

2. Ionization Data:

In a series of IAEA advisory meetings, a great deal of understanding of the important physical processes involved in ionization of ions by electrons and their data situation has been obtained. Instead of repeating the description of these processes, in Table 2 we show a summary of the present status of ionization data for typical impurities expected in plasmas. In the following comments, the pertinent literature sources for these data are summarized:

(a) He: In a June 1991 IAEA advisory meeting, the data situation has been discussed in detail[1]. The recommended data seem to be of good accuracy.

(b) Li: The recommended data have been given by Bell et al.[6].

(c) Be, B: In another June 1991 advisory meeting, detailed discussions have been presented and recommended data have been proposed by Berrington et al.[2], based largely on the scaling properties because experimental data are still scarce.

(d) C, O: Detailed discussions and recommendations have been reported in Phys. Scripta T28 (1989)[4].

(e) Ne, Ar: These gases are intended to be used for diagnostics purposes. Recommended data have been reported by Bell et al.[6] and Lennon et al.[7]

(f) Intermediate-z metallic species: The data situation has been discussed in detail for Ti, Cr, Fe, Ni and Cu in a previous 1990 advisory meeting.[4] Since then, some new data have been added.[8] However, the over-all situation seems to be largely unchanged.

TABLE 2. DATA

	ELEMENT																
Charge:	He	Li	Be	B	C	O	Ne	Ar	Ti	Cr	Fe	Ni	Cu	Ga	Mo	Ta	W
0	A	A	B	A	A	A	A	A							B		
1	A	A	C	B	A	A	A	A	B	B	B	B	B	A	B	B	B
2		A	A	C	A	A	A	A	B	D	B	C	B				
3			A	A	B	A	A	A	B	F	C	B	B			B	
4				A	B	A	A	A	D	F	C	C					
5					B	A	A	A	B	F	B	B					
6						B	B	B	D	B	B	B					
7						B	B	B	D	B	B	B					
8							B	B	D	B	B	B					
9							B	B	D	D	B	B					
10								B	D	B	B	B					
11								B	B		B	B					
12								B	C		B	B					
13								C	C	B	B	B					
14								C	C		B	B					
15								C	C		B	B					
16								C	C		C	B					
17								C	C		C	B					
18									C		C	C					
19									B		C	C					
20									B		C	C					
21									B		C	C					
22											C	C					
23											B	C					
24											B	C					
25											B	B					
26												B					
27												B					

Accuracy ratings: A=0-10%, B=10-25%, C=25-50%, D=50-100%, F = >100%

(g) Ga: This element is a candidate for a proposed liquid metal divertor system--an idea which is still in the conceptual stage. Very limited data are available so far.

(h) Heavy metallic elements: Recommended data for Mo, Ta and W have been reported only for a small number of ions of different charge states[9].

3. Excitation and Recombination Data:

The data situation is similar to that for ionization data. For the elements He, Be, B, C, O and the intermediate-Z metals, the data have been reviewed in recent IAEA advisory meetings.[1-4] Some additional excitation data for O I and O V are contained in three new papers, Refs. 10-12.

Radiative (RR) and dielectronic (DR) recombination data on various ions of the other elements of fusion interest--such as Li, Ne, Ar, Ga, Mo--may be found in a number of recent papers.[13-27]

It should be noted that recent developments of powerful ion sources and progress in accelerator technologies as well as measuring techniques have made it possible to directly determine excitation and recombination cross sections of higher ions. For example, direct measurements of excitation cross sections, using electron-ion crossed beam techniques, have been reported for Ar^{7+} and Si^{3+} ions.[28,29] Also, some recombination cross sections have been determined[30,31] based on new storage and cooling techniques in ion sources or accelerators. These techniques should soon provide systematic data for such processes involving multiply charged ions.

C. Data Requirements:

1. Spectroscopy Data:

Data are especially needed for ions of low and intermediate charge states of heavier elements. Also, the quality of transition probability data needs substantial improvements for many atomic species.

2. Ionization Data:

As seen in Table 2, more systematic studies should be devoted to very heavy elements with high melting points because there are plans for big machines such as ITER to use these materials for high heat load areas. For these heavy elements, multiple electron ionization processes should become more important than for light elements.

Also in multi-electron ions, significant fractions of the ions are often present in metastable states in the parent ion beams and show significant contributions to ionization. The recommended data should carefully take into account the effects of metastable ions in the measured data.

One should distinguish between the following, and thus provide individual cross sections for:

-- direct ionization from the valence shell
-- direct ionization from inner shells when it is important and provide branching ratios for resulting autoionizing states
-- excitation to autoionizing states plus branching ratios[32]

3. Excitation Data:

Cross sections are needed for $\Delta n > \sim 1$ transitions from metastables.

Cross sections are needed for transitions to autoionizing states with branching ratios.[32]

4. Radiative Recombination Data:

Cross sections for recombination to specific states are needed (ground state of recombined ion plus excited states which result from $\Delta n = 0$ or 1 excitations).

Approximate cross sections to higher excited states of recombined states are needed (the recombining ions may be initially in the ground or metastable states).

5. Dielectronic Recombination Data:

Cross sections or rates for specific core transitions are needed A's are the first priority. One should distinguish between the various possible $\Delta n = 0$ transitions and a single effective rate for all $\Delta n > 0$ transitions. If possible, cross sections or rates for specific $\Delta n > 0$ transitions should be determined (recombining ions may be initially in the ground or metastable states).

Finite density effects, particularly for $\Delta n = 0$ core transitions, should be evaluated.

D. Other Recommendations

1. Presentation of Data:

Analytic fits are useful, but they should always be accompanied by the tables used to generate them.

When analytic fits are provided they should, if possible, be asymptotically correct, or sensible, or a prescription should be provided to extend them outside the interval over which the fit was made. This is necessary considering the wide range of temperatures of interest to fusion.

2. Evaluation of Empirical Expressions:

The group recognizes the utility of simple empirical expressions for cross sections and rates to complement existing recommended data. Evaluations of empirical expressions should be made for the various processes of interest, and recommendations should be made.

3. Data from the Opacity Project (OP):

The working group recommends that contacts with members of the Opacity Project should be intensified, and they should be encouraged to make the results of their calculations of excitation cross sections widely available to the fusion research community.

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3.2. Working Group Report on Atomic Data Status and Needs Concerning Plasma Impurities Colliding with H, H_2 and He

D R Schultz, K Katsonis, R K Janev, Yao Jinzhang, T Shirai, V A Belyaev, V Piksaikin, H Tawara, V A Abramov, I Komarov, P Krstic and R E Olson*

I. Introduction

The present concern is the assessment of the status and needs regarding atomic collision data for impurity ion - plasma consitutuent collisions. In this regard, modelling and design relating to ITER specifically concerning the edge plasma (plasma cooling, heat and particle exhaust, plasma-wall interactions) provide one of the principal data generation, compilation and evaluation goals. This meeting focused on data for metallic (Ti, Cr, Fe and Ni) ions colliding with H, H_2 and He, but the data needed for these closely parallels that required for other impurities.

In what follows, the impurities ions of interest are categorized by nuclear charge, the reactions of greatest importance are given, recent reviews on the status of the existing data for some of these are emphasized and the specific needs identified by the present Working Group are discussed.

2. Categorization of Impurities and Reactions

The atomic impurity ions may be divided into three classes:

(i) **Low Z:** He, Li, Be, B, C, O, Ne

(ii) **Medium Z:** Al, Si, Ti, V, Cr, Fe, Ni, Cu, Ga

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* R.E. Olson did not participate in the Meeting but provided important input to the present Report

(iii) High Z: Mo, Ta, W, Tl

An obvious subset of these is also referred to as metallic impurity ions. The list includes not only impurities sputtered from the plasma confinement vessel, but those introduced for neutral beam heating, or diagnostic purposes as well. The charge states of interest include neutral ($q=0$) to fully stripped ($q=Z$) low Z ions, and charge states to at least $q=10$ for the medium and high Z cases. The energy range extends from approximately 100 eV/u in the plasma wall region to on the order of 1 MeV/u for neutral beam heating or during D-T operation.

The collisional reactions of interest are excitation, ionization and charge transfer. In addition, since collisions between plasma consitituents and partially stripped impurity ions involve possibly many electrons, processes such as radiative and Auger relaxation after impact excitation or charge transfer to multiply excited states are important. Also, needs have been identified for more information concerning collisions of metastables with impurities since such processes may have large cross sections and since metastable lifetimes may be comparable to the collision times and radiative rates characteristic of the edge plasma. State selective charge transfer cross sections are needed, most importantly for diagnostic studies, primarily for partially stripped ions colliding with H, He and H_2.

3. Recent Reports on Impurities

Several recent works coordinated by the IAEA A+M Data Unit have provided surveys of the status and needs concerning specific impurity ion classes. They include (i) a Specialist's Meeting proceedings on carbon and oxygen collision data [1] and a compilation and critical evaluation of state-selective capture in C^{6+} and O^{8+} collisions with atomic hydrogen [2], (ii) an Advisory Group Meeting proceedings on the metallic ions [3], (iii) a Working Group Report on collisional processes involving helium and helium ions [4], and

(iv) a Working Group Report on Be and B ions colliding with H, H_2 and He [5].

4. Conclusions of present Working Group

Because the number of ion species and reaction channels is so large, methods to fill in the gaps in the available experimental and theoretical data should be identified. The present Working Group has concluded that continued use should be made of both semi-empircal scaling laws [6] and scalings which result from specific theoretical models. In addition, particular theories should be applied which satisfy the requirements of sufficient reliability and computational feasiblity when confronted with the large body of data required. For example, the method of identifying hidden crossings of the branches of adiabatic energy surfaces in the complex plane [7,8] was shown to provide a useful description of excitation and ionization in slow collisions of fully stripped ions with atomic hydrogen which was much more computationally economical than other standard approaches. Therefore, such an approach could be used to provide coverage of a much larger number of collision systems than other methods. Unfortunately, almost no experimental data are available at present to test theory at low energies.

Also, a large number of calculated ionization and charge transfer total cross sections have been produced in the energy range of 10 to 1000 keV/u for Ti, V, Cr, Fe, Ni and Cu ions colliding with H, surveying these processes and demonstrating the utility of the classical trajectory Monte Carlo (CTMC) technique [9]. The CTMC method used treats the collision of these ions with simple targets as a three body collision (projectile ion, target core and target electron) in which the projectile ionic core is represented by a model potential. Such a treatment [10] was shown to be reasonable when ionization of the projectile is negligible (i.e. highly stripped ions) and when capture does not proceed to occupied, but unmodelled, shells. Thus, caution was emphasized in applying the model for low energy collisions, especially those involving low q ions. It was also demonstrated that for the medium Z impurities, this model shows essentially no Z dependence of the electron removal cross sections at a constant q, because the model potentials used vary so smoothly with nuclear and ionic charge, implying that a simple scaling could be used at the present level of approximation. Also, problems associated with autoionizing double capture were also discussed for H_2 and He targets, along with elaborations of the technique designed to go beyond these limitations. These considerations underscored the interplay and balance between the specific fusion plasma modelling needs and the robustness or level of approximation necessary to assure computational efficiency and theoretical tractability.

In general the greatest needs exist for collisional data concerning low energy ($E \leq 100$keV/u), low charge state ions ($q \leq Z^{1/2}$). Such collisions are clearly the most challenging theoretically because of the large number of final states and the many-electron effects which must be treated. In addition, this collision regime does not often allow representation of the data by scaling relations and therefore experimental benchmarks are urgently needed. Further, while progress has been made in data production for low and medium Z impurities, very little data exists for the high Z impurities, or for collisions involving excited state target species. A continued role of the A+M Data Unit in coordinating efforts to generate and evaluate ion-atom collisional data involving impurity ions is essential.

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6 T Shirai, contribution to this meeting

7 I Komarov, contribution to this meeting

8 P Krstic, contribution to this meeting

9 K Katsonis, contribution to this meeting

10 D R Schultz, contribution to this meeting

4. MEETING CONCLUSIONS AND RECOMMENDATIONS

The detailed analysis of the existing atomic data and the data needs for fusion plasma impurities, performed during the Working Group sessions and discussed at the concluding plenary session of the Meeting, can be summarized as follows:

1) The spectroscopic data base (energy levels, wavelengths, transition probabilities) for plasma impurities with $Z \leqq 10$ is virtually complete and of very high quality (accuracies $< 5\%$, with few exceptions). With increasing Z, both the completeness and quality of the data deteriorate, becoming moderate for the impurities with $10 < Z \leqq 30$ (but the accuracy remaining still high) and fragmentary for $Z > 30$ (accuracy is good only for energy levels and wavelengths). In general, the energy level and wavelength data are an order of magnitude more accurate than those for transition probabilities. Improvement of the data on transition probabilities for many medium-Z impurities is required, as well as generation of new, presently not available, spectroscopic data for the high-Z impurities (Mo, Ta, W).

2) The status of data bases for electron-impact processes of several groups of low- and medium-Z plasma impurities (He, Be, B, C, O, Ti, Cr, Fe, Ni, Cu) has been reviewed by several recent experts' groups at the IAEA. The conclusions and recommendations of those groups remain valid also at the present time. Regarding the high-Z impurities (Mo, Ta, W), the collisional data bases for excitation, ionization (including multiple) and recombination are in rather unsatisfactory state, particularly for the ions in low charge states. A substantial increase of data generation activity for these elements is required, which could be one of the dominant tasks for the recently initiated IAEA Co-ordinated Research Programme on A+M data for medium- and high-Z impurities. The electron-impact collisional data bases for plasma diagnostic impurities (such as Ne, Ar, Ga) is also rather sparce (particularly for Ga) and its completion requires a major co-ordinated effort.

3) The data base for collision processes (excitation, ionization, electron capture) of plasma impurity ions with the plasma edge neutrals (H, H_2, He) is still in a very fragmentary state and, generally speaking, of moderate accuracy. The lack of reliable data is particularly noticeable for ions in

low charge states and for collisions in the low (< 1 keV/amu) energy region, relevant for the plasma edge studies. For certain applications, where only high-energy data of completely stripped ions are required (such as H- and He-beam injection), the data base for heavy-particle collision processes is in much better shape. Large-size molecular-orbital coupled channel calculations are necessary for generating accurate low-energy data for the heavy-particle collision processes. In the case of one-electron collision systems, a systematic application of the recently developed adiabatic superpromotion model is strongly encouraged. For data generation in the intermediate-to-high energy collisions of incompletely stripped ions with H, H_2 and He, apart from the atomic-orbital (+ pseudostates) close-coupling method, a wider application of the CTMC method is encouraged, with due attention to the problem of effective potentials and a possible extension of the method beyond its present Hamiltonian formulation. A workshop on these subject, organized by either the IAEA or one of the most active CTMC computation groups, would be highly desirable.

4) There is a need for systematic up-dated calculations of the radiative cooling rates of plasma impurities, paralleling the improvements (in terms of completeness and quality) in the radiative and collisional data bases for each individual plasma impurity. The results for the carbon and oxygen impurities presented at this meeting are a good beginning. The ultimate goal of such calculations is to be performed within a radiative-collisional plasma model, but even partial steps in this direction (such as explicit inclusion of metastables, or a limited number of low-lying states) would be very useful. Establishment of a recommended data base for the impurity cooling rates should be one of the priorities in the future IAEA fusion related A+M data activities.

Appendix 1

IAEA Advisory Group Meeting on "Atomic and Molecular Data for Fusion Plasma Impurities"

25 - 27 September 1991, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Advisory Group Meeting on "Atomic and Molecular Data for Fusion Plasma Impurities"

25 - 27 September 1991, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

WEDNESDAY, September 25

09:30 - 09:45 - Opening (Room: C07-IV)
- Adoption of Agenda

Session 1: Spectroscopic and electron-impact collision data

Chairman: H. Tawara

09:45 - 10:15 W.L. Wiese: Spectroscopic data for fusion plasma impurities

10:15 - 11:15 A.Ya. Faenov: Plasma impurity spectroscopic data bases and activities at VNIIFTRI

11:15 - 11:30 Coffee break

11:30 - 12:00 L.A. Vainshtein: Code ATOM for calculation of atomic characteristics and processes

12:30 - 14:00 Lunch

Session 2: Data for heavy-particle collisions

Chairman: V.A. Abramov

14:00 - 14:30 D.R. Schultz: Classical Trajectory Monte Carlo (CTMC) calculations for plasma impurity collisions

14:30 - 15:00 K. Katsonis: CTMC cross section calculations for electron capture and ionization in collisions of plasma impurity ions with He

15:00 - 15:30 Coffee break

15:30 - 16:00 H. Tawara: Data needs for electron transfer processes of MeV positive and negative heavy ions for electromagnetic field measurements in plasmas

16:00 - 16:30 T. Shirai: Data activities on fusion plasma impurities at JAERI

THURSDAY, September 26

Session 3: Data for heavy-particle collisions and plasma application

Chairman: W.L. Wiese

09:30 - 10:00 I.V. Komarov: Simple estimates for ionization of hydrogen-like ions by slow bare nuclei due to superpromotion

10:00 - 10:30 P. Krstic: Calculations of excitation and ionization cross sections for He^{2+}-H slow collisions

10:30 - 11:00 Coffee break

11:00 - 11:30 V.A. Abramov: Calculations of the cooling rates for a Mo - seeded plasma

11:30 - 12:00 R. Marchand: Radiative and electron-energy losses associated with plasma impurities

12:30 - 14:00 Lunch

Session 4: A+M data status and needs for fusion plasma impurities

Chairman: R.K. Janev

14:00 - 15:00 General discussion on the A+M data status and needs for plasma impurities:

- Completness and quality analysis of the existing database and priorities in data generation;
- Establishment of working groups for detailed data status analysis.

15:00 - 15:15 Coffee break

15:15 - 17:00 Working Group Sessions

1. Working Group on Spectroscopic and Electron-Impact Collision Data (Room: C-0739)
2. Working Group on Heavy-Particle Collision Data (Rm: 07-IV)

FRIDAY, September 27

Session 4:	(Cont'd)
09:30 - 12:00	Working Group Sessions Preparation of Working Group Reports, conclusions and recommendations
12:00 - 14:00	Lunch
Session 5:	Meeting conclusions and recommendations
Chairman:	R.K. Janev
14:00 -16:00	- Discussion and adoption of Working Group Reports - Formulation and adoption of Meeting conclusions and recommendations

Appendix 3

Data needs for electron transfer processes of MeV heavy (positive and negative) ions, applied to electro-magnetic field measurements in plasmas

H. Tawara

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It is important to know the electro-magnetic fields inside plasmas. In particular the potential and its (temporal as well as spatial) distributions could play a crucial role in determining features of plasmas such as turbulences. Among the proposed methods to measure the potential in plasmas, heavy ion beam probe (HIBP)[1] could be a promising technique as this could give information on spatial and temporal dependence of the plasma potential. Its working principle is based on measurements of the energy variation of heavy ions injected into a plasma which is charge-changed through collision with plasma constituents.

Because of the limited space available near plasma apparatus, some requirements for the HIBP system have to be fulfilled :
a) over-all system should be of moderate size, b) the deflection of ions in magnetic fields (a few Teslas) should not be too large, c) high energy stability (10^{-5}) of the ion beams is required as the potential in plasmas is expected to be on the order of 1 kV.

After taking into account these requirements, a proposed HIBP system at NIFS[2] would consist of the following elements (see Fig.1) :

a) Negative heavy ion beams (Au, Tl, Bi, for example) are injected into a tandem electrostatic accelerator with positive (1-3) MV terminal voltage.
b) Negative ions of (1-3) MeV are stripped to positive ions with the charge of q = 2-4 through collisions with gas at the terminal.
c) After selecting appropriate final energy of (5-10) MeV, ions collide with gas targets and capture some electrons.
d) Before injecting into a plasma, singly charged ions are selected.
e) Some of the injected singly charged positive ions collide with plasmas and change the charge as well as the energy which depends upon the plasma potential at the collision region. Then they gain or lose the energy. This

energy change give us information of the potential inside plasmas.

Thus, in this system, the important collision processes are categorized into the following three types :

1) (1-3) MeV negative ion collisions with neutral gas
2) (5-10) MeV positive ion collisions with neutral gas
3) (5-10) MeV singly charge ion collisions with plasma.

As known already in many collisions of ions, the important parameter is ratio of the ion velocity to the orbital velocity of electrons under consideration, v_i/v_e. At small ratios, the dominant process is the electron capture, whereas the electron stripping becomes dominant at large ratios.

The corresponding important collisions in the proposed HIBP system are divided as follows$^{3)}$:

1) (5-15 keV/amu) negative ion collisions with gas

$$A^- + B \rightarrow A^{q+}$$

As the binding energy of an additional electron in negative heavy ions is 0.1-1 eV, the velocity ratio above is roughly 5-10. This suggests that the stripping (or detachment) of this loosely bound electrons is dominant. The data status of negative ion collisions has been summarized recently by Rahman and Hird$^{4)}$. However, they covered those only for single and double electron stripping of ions up to I^-. The knowledge of equilibrium charge distributions at the MeV energy region can be obtained from a compilation by Shima et al.$^{5)}$

There could be some empirical scaling formulas for single electron stripping processes from negative ions, similar to the Lotz formula for ionization of ions or atoms by electron impact. However, there seems no simple scaling for multiple electron stripping processes.

2) (30-60 keV/amu) positive ion collisions with gas

$$A^{q+} + C \rightarrow A^{(q+i)+}$$
$$\rightarrow A^{(q-i)+}$$

As the binding energy of multiply (low) charge state ions is 15-50 eV, the above ratio is roughly unity where electron capture and loss processes compete each other. And multiple electron processes may also play a role. The data status was summarized by Dehmel et al.$^{6)}$ who covered the electron stripping cross sections of neutral and singly charged ions up to U^+ ions of 1 MeV and Ho & Fite$^{7)}$ who covered single electron capture and multiple electron stripping of singly charged ions (as well as of a limited number of doubly charged ions) including MeV U^+.

For single electron capture processes, a number of scaling formulas have been proposed. For example, Knudsen et al. proposed the following formula including the effect of different target gas[8)], based upon the Bohr classical idea :

$$\sigma_{q,q-1} * z^{2/3} \sim E_i/(q^{4/7} * z^{16/21}).$$

where z is the atomic number of target and E_i the ion energy. This is valid for q >_ 5. The scaling properties of this formula can be seen in Fig.2. For low charge (< 3-4), strong oscillations of the cross sections have been observed. Also at this energy region, there are some anomalies such as oscillation around smooth q-dependence[9] or dips around the closed shell. However, the variations are within a factor of 2-3.

Only a limited data are available for multiple electron capture processes.

Similarly some empirical scaling formulas have been proposed to estimate the electron stripping cross sections. Dmitriev et al. found that the cross sections for single electron loss can scale as follows[10)] :

$$\sigma_{q,q+1} \sim (n_e * z^n / E_e^m) * f(E_i/E_e)$$

where n_e represents the number of electrons in the outer shell, E_e the binding energy of an electron (m = 1.3), z the effective nuclear charge of target (empirically n~ 2/3). As shown in Fig.3, experimental data are scattered at low E_i/E_e (v_i/v_e) region around this scaling. Note that this scaling is based upon mostly light ions.

Only a limited data are available for multi-electron stripping processes.

3) (30-60 keV/amu) positive, singly charged ion collisions with plasma

$$A^+ + \text{plasma} \rightarrow A^{2+}$$

As the binding energy for singly charged ions is roughly 10-20 eV, the ratio discussed above are about 10-20 where the electron stripping processes are expected to become dominant. However, so far no systematic investigations have been performed in plasma targets at the present energy region. As protons are assumed to be the most dominant constituent, collisions of heavy ions with protons as target could be studied experimentally[11)] :

$$A^+ + H^+ \rightarrow A^{q+}.$$

Urgent data needs

As seen above, some empirical scalings or calculating formulas[12)] can be used to know the cross sections at least for single electron processes. However, there seems no simple scaling for estimating the cross sections of multi-electron processes for relatively low charge with intermediate energy region which seem to be relevant to HIBP. The following data are needed for designing the efficient HIBP system :

1) $\sigma_{-1,q}$ for (5-15 keV/amu) heavy negative ions in gas
2) $\sigma_{q,q'}$ for (30-60 keV/amu) heavy positive ions in gas
3) $\sigma_{1,q}$ for (30-60 keV/amu) singly charged heavy ions in plasma

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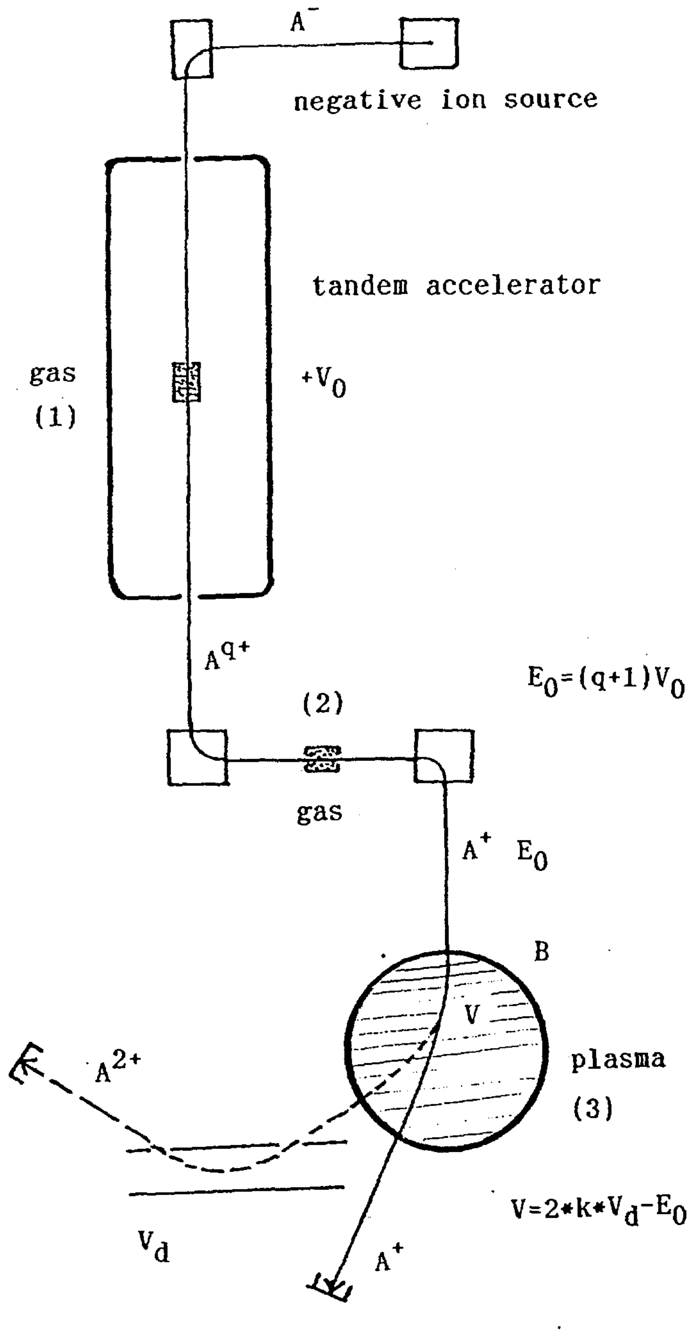

Fig.1 A scheme for measuring potential in a plasma

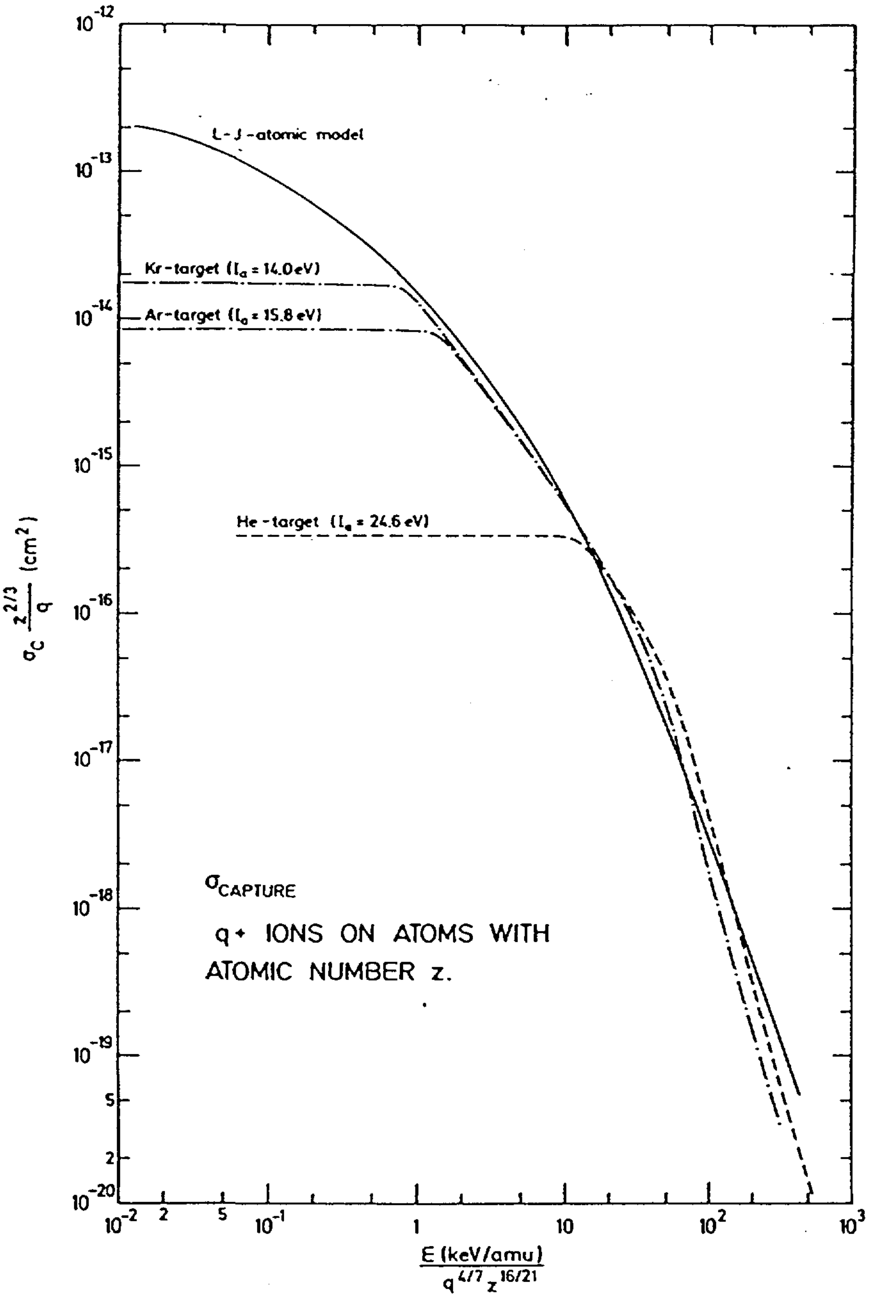

FIG. 9. The electron-capture cross section found from Eq. (27), which is based on the Bohr-Lindhard cross sections and the Lenz-Jensen atomic model. It is compared to the results for He, Ar, and Kr targets obtained from the simple estimate [Eq. (17)].

Fig.2 Scaling properties of single electron capture proposed by Knudsen et al.

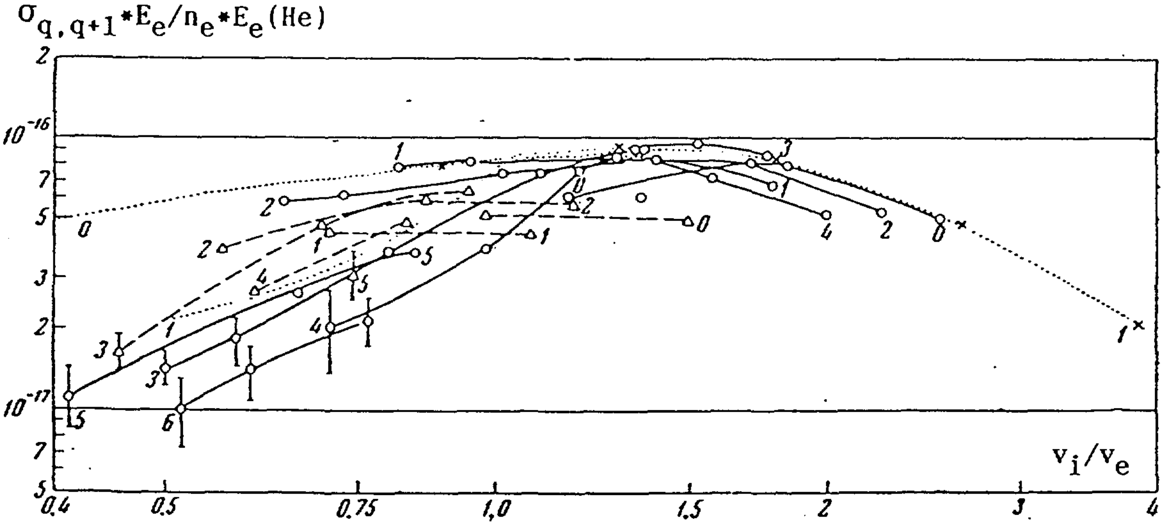

FIG. 8. Dependence of $\sigma_{i,\ i+1} I/qI_0$ on v/u for He (x), N (o) and Ne (Δ) ions in helium (I_0 = 13.5 eV). The values of i are marked by the curves. The values of σ_{01} for helium atoms were taken from Allison's review.[1]

Fig.3 Scaling of single electron stripping of He, N and Ne ions in helium target proposed by Dmitriev et al.

Appendix 4

A+M Data Needs for the Neutral Beam Heating System for Next-Step Fusion Devices

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The next-step fusion devices, as exemplified by the International Thermonuclear Experimental Reactor (ITER) will require injection of powerful (80-100 MW) and energetic (0.5 - 1 MeV/amu) neutral deuterium beams for plasma heating and current drive in the central plasma region. The performance optimization of neutral beam injection system requires accurate atomic collision data bases for the following areas:

1) Atomic processes in the D^- ion source

The D^- ion source is a hydrogen discharge (with an appropriate admixture of alkalies or earth-alkalies) with a plasma temperature in the range of several eVs.

The important processes which determine the D^- production of the source are:

a) Electron-impact and ion (atom)-molecule collision processes involving D^o, D^+, D_2^o, D_3 and D_2^+ in their ground and ro-vibrationally excited states, particularly the processes leading to formation and distruction of D^-.

b) Atomic collision process with surfaces of the ion source leading to change of the charge and quantum state of atomic and molecular particles and to formation or distruction of D_2^+, D_2 and D^-, as function of the surface temperatures and for various surface materials and layers.

c) Specific processes for diagnostics of the ion source plasma.

2) Atomic processes along the beam line

a) Atomic processes in the negative ion beam neutralization chamber of 0.5 - 1 MeV/amu D^- ions with the particles of the neutralizer plasmas (of different composition (Ar, Kr, Xe) and at various degrees of ionization).

b) Collision processes between the beam particles due to the beam energy spread (both in the negative ion and neutralized beam).

c) Charge changing processes of D^+ and D^- ions (energy: 0 - 1 MeV/amu) colliding with a cooled coper surface at different (including grazing) incidence angles.

3) Atomic processes of energetic D^0 atoms (0.5 - 1 MeV/amu) with reactor plasma constituents

Most of these processes have already been documented in previous IAEA activities. Some improvement of the corresponding data base is desirable for the excitation processes involving impurity ions and for transitions between excited states.