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IAEA ADVISORY GROUP MEETING ON

"ATOMIC AND MOLECULAR DATA FOR METALLIC IMPURITIES IN FUSION PLASMAS"

Vienna, 16-18 May, 1990

SUMMARY REPORT

Prepared by R.K. Janev

July 1990

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

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Abstract

The present Report contains the Summary of the IAEA Advisory Group Meeting on "Atomic and Molecular Data for Metallic Impurities in Fusion Plasmas" which was organized by the IAEA Atomic and Molecular Data Unit and held on May 16-18, 1990 in Vienna, Austria. The Meeting Proceedings are briefly described and the Working Group Reports on electron impact and heavy particle collisions are reproduced. The meeting conclusions regarding the data status and the recommendations for future IAEA activities in this data area are also included.

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1. INTRODUCTION

Following a recommendation of the Subcommittee on Atomic and Molecular (A+M) Data for Fusion of the International Fusion Research Council (IFRC Subcommittee), given at its 5th Meeting (October 7-8, 1988), the IAEA Atomic and Molecular Data Unit convened on May 16-18, 1990, an Advisory Group Meeting (AGM) on "Atomic and Molecular Data for Metallic Impurities in Fusion Plasmas" at the IAEA Headquarters in Vienna.

The Meeting objectives were:

1) to review the A+M data status for the most important fusion plasma metallic impurities (Ti, Cr, Fe, Ni);
2) to identify the gaps in the database, particularly for the most important collision processes; and
3) to formulate appropriate conclusions and recommendations regarding the status and immediate and longer-term data generation and evaluation activities for metallic impurities, in order to conform with the needs of the fusion research and reactor design work.

The data for the following categories of collision processes were analyzed:

a) Collisions of electrons with metal impurity ions A^{q+} (A=Ti, Cr, Fe, Ni).
   Processes: excitation, ionization, radiative and dielectronic recombination.
b) Collisions of the impurity ions A^{q+} with H, H_2 and He.
   Processes: total and state selective electron capture, ionization, excitation, dissociative processes (in case of H_2).

In the preparatory stage of the Meeting, a large number of potential participants and experts from the atomic physics community were asked to prepare reviews on the data status for specific types of processes (including data quality assessment) and to perform theoretical calculations or experimental measurements for specific processes and collision systems. The response to this action has been unusually positive, resulting in a thorough coverage of the existing database and in generation of a significant amount of new data, reported for the first time at the Meeting. Invited contributors who were not able to attend the meeting have sent their contributions to the meeting, or will send them for publication in the Meeting Proceedings (to be published as a Topical Issue of "Physica Scripta").

The meeting was attended by 18 participants (4 from the IAEA), covering almost uniformly the various collision processes, energy ranges and research methods (theoretical and experimental). The List of Participants is given in Appendix 1.

2. MEETING PROCEEDINGS

The Meeting was opened by Dr. J.J. Schmidt, Head of the IAEA Nuclear Data Section, and then its work proceeded in seven sessions. The Meeting Agenda is given in Appendix 2.

The working sessions of the meeting were:

1) Electron-ion collisions: Recombination,
2) Electron-ion collisions: Excitation and ionization,
3) Heavy-particle collisions: Experimental and quantum-mechanical results,
4) Heavy-particle collisions: CTMC results,
5) General discussion of atomic database for metallic impurity ions,
6) Data evaluation and preparation of Working Group Reports,
7) Discussion of Working Group Reports and adoption of AGM recommendations.

Below, we briefly describe the highlights of presentations and discussions in the sessions.

In the session on electron-ion recombination, Y. Hahn presented exhaustive numerical information on the dielectronic recombination (DR) rates for the A^{q+} (A=Ti, Cr, Fe, Ni) ions in the field free/zero-density case. He also presented analytic formulae for the radiative recombination rate, with an appropriate assessment of their validity. N. Badnell presented DR rates for a number of Fe^{q+} ions (q=15, 21, 22, 23, 24, 25) and discussed the inclusion of the plasma density effects. M. Bitter presented experimentally determined DR rates for He-like TiXXI, FeXXV, NiXXVII and H-like TiXXII ions at temperatures typical for the TFTR plasmas (1-5 keV). A Müller reported on the first cross section measurements of the radiative recombination of free electrons on C^{6+} and U^{28+} ions.

In the session devoted to the electron-impact excitation and ionization of metallic impurities, D. Gregory presented a comprehensive review of the excitation processes and data, while A. Müller reviewed the data situation for ionization. The excitation-autoionization and other many-electron transition processes were also included in these presentations. R.E.H. Clark and J. Abdallah (results presented by D. Gregory) have provided to the Meeting an almost complete electron impact database for Titanium ions (calculated by a set of coupled codes (CATS, ACE, GIPPER) mainly within the DW approximation). Extensive CBE cross section and reaction rate calculations for excitation of many transitions in Ti^{q+}, Cr^{q+}, Fe^{q+} and Ni^{q+} ions were reported by V.P. Shevelko. R-matrix calculations of the collision strengths for many transitions in Fe^{q+}, (q=1-25) and Ti^{20+} were presented by K. Berrington. Ionization cross sections for Ca^{q+}, Fe^{q+} and Ni^{q+} in the Born-Oppenheimer approximation were reported by V.P. Shevelko, while N. Badnell presented ionization cross sections for the transition metal ions, calculated in higher-order approximations. V.A. Abramov provided a comparison of the electron-impact excitation data, evaluated by several groups, and demonstrated their consistency for the majority of analyzed cases.

In the session devoted to the heavy-particle collisions (experimental and quantum-mechanical results), H.B. Gilbody presented a detailed review of the experimental situation for all types of processes in the metal ion- H, H_2, He collision systems, including a review of the most important theoretical results and semi-empirical scalings. W. Fritsch presented a comprehensive set of coupled-state cross section calculations for the total and state selective electron capture in Ti^{4+}, Cr^{6+}, Fe^{8+} + H collisions. He also provided estimates for the excitation cross sections in the above collision systems. G.L. Yudin reported on a unitarized first Born theory for excitation, and presented results for the n=2 excitation of H(1s) by several multicharged A^{q+} ions (A=Ti, Cr, Fe, Ni; $6 \leqq q \leqq 14$). H. Cederquist discussed an extension of the over-barrier electron capture classical model to describe the transfer-excitation (simultaneous capture and target-product excitation).

In the session devoted to the application of Classical Trajectory Monte Carlo (TCMC) method to electron capture and ionization in heavy-particle collisions, R.E. Olson presented an extension of the method to two-electron targets and an extensive set of results for electron capture, ionization and transfer-ionization in collisions of A^{q+} with He and H_2 (including some dissociative channels in the case of H_2 target). K. Katsonis also presented a comprehensive set of cross sections for total capture, shell-selective capture, and ionization for collisions of a number of highly charged metallic ions (Al^{q+}, Fe^{q+}, Mn^{q+}) with hydrogen atoms.

The other sessions of the meeting were devoted to detailed discussions of the status and quality of the database for the metallic impurities in fusion plasmas. Two working group were formed with the task to analyze the databases in the areas of electron-ion and heavy-particle collisions. Their reports are given in the next Section of this Report. The conclusions and recommendations of the Advisory Group, adopted at the last Meeting session, are given in Section 4.

3. WORKING GROUP REPORTS

3.1. Status of the Electron-Ion Database for Metallic Impurities

D.C. Gregory, Y. Hahn, A. Müller (Co-Chairmen), V.A. Abramov,
N.R. Badnell, K. Berrington, M. Bitter, and V.P. Shevelko

1. Introduction

The available data for electron collision processes of most importance to the fusion community are evaluated and referenced in this summary for collisions involving the primary metallic impurity elements found in present and near-future fusion devices. Recommendations are made concerning work needed in the future to fill in gaps and to complete our basic understanding of the important processes involving these impurity elements.

2. Ionization

The status of available specific data on electron impact ionization for the impurity elements of immediate interest to the fusion community is summarized in Table 1. References are listed at the end of the table, and the letter designations refer to the accuracy of the reference data (according to the ALADDIN evaluation scheme, which is also given at the end of the table). Accuracy ratings are for ions in equilibrium plasmas, in the energy range from threshold to roughly three times threshold. Copper has been included up to 3+ to provide a tie-point for interpolation of data to nearby elements.

The two processes leading to ionization which are considered to be of primary importance are direct ionization and excitation-autoionization. Rates based on the sum of these cross sections are adequate for the needs of the fusion community. Where only direct ionization calculations are available, the accuracy given in Table 1 includes consideration of the expected influence of excitation-autoionization.

In some cases the actual rate coefficients may be 10% higher than the sum of direct ionization and excitation-autoionization due to resonant effects (such as REDA), usually only in limited energy ranges near major excitation features. Accurate total ionization calculations including resonant processes are available only for a few ions in the Li and Na isoelectronic sequences, and a large number of such accurate theoretical studies are not expected in the future.

Multiple ionization will be important at energies several times the threshold energy. In equilibrium plasmas, a given ionization stage will normally have been "burned-through" before reaching the plasma region dominated by these high temperatures, but multiple ionization should be considered when dealing with ions at temperatures far above their equilibrium range.

The excitation and ionization cross sections needed to calculate accurate total ionization rates are available for the complete Ti isonuclear sequence, but the job of combining these cross sections and calculating the appropriate total ionization rates has only been carried out for a few charge states of Ti.

The referenced calculations for Fe ions above charge state 15+ (Na-like) include only direct ionization. It is not obvious that excitation-autoionization will be negligible for all higher charge states.

Experimental plasma rate measurements are available for some Ti and Fe charge states above 15+. However, these results are somewhat model dependent, have large uncertainties, and are usually measured at only one or two temperatures. The relatively poor accuracy ratings reflect these uncertainties.

Table 1: Electron Impact Ionization

	Ti		Cr		Fe		Ni		Cu
Charge	E	T	E	T	E	T	E	T	E
0	–	–	–	–	B	–	–	–	B
1	B	D	B	D	B	C	B	C	–
2	B	B	–	D	B	C	–	C	B
3	B	F	–	F	–	C	B	C	B
4	–	D	–	F	–	C	–	C	
5	B	B	–	F	B	B	B	B	
6	–	D	B	D	–	B	B	B	
7	–	D	B	D	–	B	B	B	
8	–	D	B	D	–	B	B	B	
9	–	D	–	D	B	B	–	B	
10	–	D	B	D	–	B	–	B	
11	B	B	–	–	B	B	–	B	
12	–	C	–	–	–	B	B	B	
13	–	C	B	–	B	B	–	B	
14	–	C	–	–	–	B	B	B	
15	–	C	–	–	B	B	–	B	
16	F	C	–	–	F	C	–	B	
17	F	C	–	–	F	C	–	B	
18	F	C	–	–	F	C	–	C	
19	F	B	–	–	F	C	–	C	
20	–	B	–	–	F	C	–	C	
21	–	B	–	–	F	C	–	C	
22			–	–	–	C	–	C	
23			–	–	–	B	–	C	
24					–	B	–	C	
25					–	B	–	B	
26							–	B	
27							–	B	

E=Experiment T=Theory –=None available

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

References for Table 1

(nE or nT designates an E or T data source for the n-th charge state)

Titanium
EXPERIMENT: (1E,2E) J. Phys. B 21, 2129 (1988); (3E) Phys. Rev. A 27, 762 (1983); (5E) Phys. Rev. A 41, 140 (1990); (11E) Phys. Rev. A June 1990; (16-19E) Phys. Rev. A 33, 4293 (1986).
THEORY: (1T,4T,6-10T,12-21T) R.E.H. Clark and J. Abdallah, Jr., proceedings of this meeting; (2T) ; (5T) Phys. Rev. A 41, 140 (1990); (11T) Phys. Rev. A 36, 3642 (1987).

Chromium
EXPERIMENT: (1E) J. Phys. B 20, 2571 (1987); (6-8E,10E) Phys. Rev. A. 39, 2397 (1989); (13E) Phys. Rev. A June (1990).
THEORY: (1-10T) V. Shevelko, proceedings of this meeting.

Iron
EXPERIMENT: (0E) Phys. Rev. A 41, 3575 (1990); (1E) J. Phys. B 17, 2085 (1984); (2E) Phys. Rev. A 31, 2905 (1985); (5E,6E,9E) Phys. Rev. A 34, 3657 (1986); (11E,13E,15E) Phys. Rev. A 35, 3256 (1987); (16-21E) Phys. Rev. A 38, 4761 (1988).
THEORY: (1-25T) "Electron Impact Ionization Data for the Iron Isonuclear Sequence", by M.S. Pindzola et al., ORNL/TM-10297 and Nuclear Fusion 1987 Special Supplement, Recommended Data on Atomic Collision Processes Involving Iron and Its Ions, pp. 21-41; (15T) Phys. Rev. Lett. 64, 1350 (1990).

Nickel
EXPERIMENT: (1E) J. Phys. B 18, 1419 (1985); (3E) Phys. Rev. A 34, 97 (1986); (5-8E,12E,14E) J. Phys. B 21, 2117 (1988).
THEORY: (1-27T) "Electron Impact Ionization Data for the Nickel Isonuclear Sequence", by M.S. Pindzola et al., ORNL/TM-11202 and proceedings of this meeting.

Copper
EXPERIMENT: Phys. Rev. A 41, 3575 (1990); (2E,3E) Phys. Rev. A 34, 97 (1986).

3. Excitation

There are no direct experimental measurements of electron impact excitation of the ions of primary interest to this report. The extremely large number of possible transitions for all charge states of the elements of interest precludes a specific evaluation of calculations for each transition. An accuracy rating of "C" is assigned to the Coulomb-Born (with exchange) calculations by V.P. Shevelko for Ti, Cr, and Ni ions (charges 1+ through 9+) which are included as part of the complete report of this meeting (to be published as a Topical Issue of "Physica Scripta" by the end of 1990). Distorted-wave excitation calculations for inner- and outer-shell electrons for all charge states of Ti are described by Clark and Abdallah, and will appear also in the complete report of this meeting. These calculations receive a "B" rating. Other calculations are available in the literature. The Opacity Project has complete calculations of excitation cross sections for Fe charge states 1+ and 23+, and fairly complete results for 2+ to 4+ (for the time being, availability should be discussed with project members).

Resonant excitation is very important for non-dipole-allowed transitions. The net effect ranges from a slight decrease in cross section to 500% enhancements and extends over wide energy ranges.

The bulk effects of numerous inner-shell excitations to autoionizing states have been tested for a wide range of charge states and elements through ionization measurements. The good agreement observed in most cases gives us confidence that inner-shell excitation calculations are reasonably accurate.

4. Radiative Recombination

Radiative recombination is less important in plasmas than dielectronic recombination for all isoelectronic sequences except H-like and He-like ions. The distorted-wave calculations of radiative recombination for Fe and Ti ions included in the complete report are assigned an accuracy level of "B".

Accelerator-based radiative electron capture (REC) measurements, employing ion-atom collision processes analogous to radiative recombination, generally support (within their limited accuracies) radiative recombination calculations.

5. Dielectronic Recombination

Table 2 summarizes the available data on dielectronic recombination for the impurity elements of primary interest in this report. References are included and accuracy ratings are given. All data are for total rate coefficients at zero density and target ions in their ground state. Density and field effects are important in plasmas and must be considered in order to obtain realistic rates for use in plasma modelling.

Limited calculations are available for $\Delta n>0$-transitions in Li-like ions. Dielectronic recombination rates for Ti ions could be calculated based on the information available in the paper by Clark and Abdallah which will appear in the complete Meeting Proceedings ("Physica Scripta", Topical Issue), but such calculations would fall in categories "B" and "C".

The limited number of experiments available from EBIT and line ratio measurements generally compare well with theory. Excitation followed by radiative decay (RTEX) measurements also support theory within the limited precision and accuracy of those measurements. Detailed experiments (from Aarhus and Heidelberg) on DR of C, N, O ions for $\Delta n=0$-transitions and on $\Delta n \geqq 1$-transitions in O^{7+} also compare well with calculations.

Table 2: Dielectronic Recombination

Initial no. of electrons	Ti		Cr		Fe		Ni	
	E	T	E	T	E	T	E	T
1	-	B	-	-	-	B	-	B
2	-	B	-	B	B	B	B	B
3	-	-	-	-	-	B	-	-
4	-	B	-	B	-	B	-	B
5	-	-	-	-	-	B	-	-
8	-	-	-	-	-	F	-	-
9	-	-	-	-	-	B	-	-
10	-	B	-	B	-	B	-	B
11					-	C		
12					-	C		
...								
21	B	-					-	-

E=Experiment T=Theory -=None available
Accuracy ratings: A=0-10% B=10-25% C=25-50% D=50-100% F= >100%

References for Table 2

(kT or kE designates respectively a T or E data source for ion with k electrons)

Titanium

Theory: (1T) Phys. Rev. A 37, 2599 (1988); (2T) Phys. Rev. A 33, 994 (1986); (4T) J. Phys. B 20, 2081 (1987); (10T) Phys. Rev. A 34, 1073 (1986). (21E) Phys. Rev. A 29, 661 (1984).

Chromium

Theory: (2T) Phys. Rev. A 39, 3548 (1989); (4T) J. Phys. B 20, 2081 (1987); (10T) Phys. Rev. A 34, 1073 (1986).

Iron

Experiment: (2E) Phys. Lett. A 93, 189 (1983).
Theory: (1T) Phys. Rev. A 37, 2599 (1988); (2T) Phys. Rev. A 39, 3548 (1989); (3T) Phys. Rev. A 29, 712 (1984); (4T) J. Phys. B 20, 1081 (1987); (5T) J. Phys. B 19, 3827 (1989); (8T) Phys. Rev. A 35, 3368 (1987); (9T) Phys. Rev. A 34, 1079 (1986); (10T) Phys. Rev. A 34, 1073 (1986); (11T) Phys. Rev. A 30, 316 (1984); (12T) JQSRT 38, 311 (1987).

Nickel

Experiment: (2E) Phys. Rev. Lett. 62, 2104 (1989).
Theory: (1T) Phys. Rev. A 37, 2599 (1988); (2T) Phys. Rev. A 39, 3548 (1989); (4T) J. Phys. B 20, 2081 (1987); (10T) Phys. Rev. A 34, 1073 (1986).

6. Metastable Ions

The presence of metastable ions can be very important in considering the power balance in a plasma. Dielectronic recombination and, in some cases, ionization cross sections can be quite different for metastables when compared to the ground state of the same ion. It is currently quite difficult to predict (or often to measure) the presence or percentage of metastables to be found for a given ion in a given plasma. Once the presence and percentage is established, the physics of the metastable ion can generally be understood, given appropriate consideration and attention.

7. Gaps in the database

a) IONIZATION - For electron impact ionization, some gaps in the data do exist, as can be seen from Table 1. However, these gaps can generally be filled by calculations or interpolation along isoelectronic sequences from nearby known values. A number of measurements are needed for highly charged ions (with 10 or fewer electrons) to establish the importance of excitation-autoionization and the accuracy of direct ionization for these isoelectronic sequences.

b) EXCITATION - Measurements of direct excitation are needed. There are several research efforts under way to provide such measurements, and these results will be important to test various aspects of existing and future excitation calculations. It has been stated that resonant excitation for non-dipole-allowed transitions can be very important indeed. More work and a better understanding of the systematics of this phenomena are greatly needed.

c) RADIATIVE RECOMBINATION - Direct accurate measurements are needed. The only published measurement to date is in good agreement with theory, but other preliminary measurements show large discrepancies. RR is important not only because of direct plasma applications, but also because other important atomic physics measurements are normalized to RR calculations. For plasma modelling applications, Cr and Ni data may be interpolated from other existing calculations. For lower charge states, the accuracy is less important because the models are less sensitive to RR rates.

d) DIELECTRONIC RECOMBINATION - Measurements and calculations are needed for 6-, 7- and 8-electron systems for these elements. There are also no published data for systems with more than 12 electrons for the impurity elements. For the many-electron systems, only a factor of two accuracy is needed, and this should be achievable. A simple formula is needed to allow adjustment of the zero density DR rates as a function of charge and field for a given temperature. Existing formulas are not adequate for the densities found in fusion plasmas. We exclude consideration of very high densities here.

e) METASTABLES - An overall better understanding of metastables is needed. A general diagnostic which could identify and quantify the presence of metastable ions in a plasma device or in a beam extracted from such a device would be most helpful.

3.2. Collisions of H, H_2 and He with Metallic Impurity Ions

W. Fritsch, H.B. Gilbody, R.E. Olson (Joint Chairmen)
H. Cederquist, R.K. Janev, K. Katsonis and G. Yudin

1. Introduction

The reactions of relevance to a better understanding of the physics of the plasma edge and to neutral beam diagnostics may be summarized as follows:

For atomic hydrogen targets, cross sections for total charge transfer (which includes all final bound states of the product ion)

$$X^{q+} + H \rightarrow X^{(q-1)+} + H^+$$

and for state selective capture in which the (n,ℓ) product state is specified

$$X^{q+} + H \rightarrow X^{(q-1)+}(n,\ell) + H^+$$

ionization

$$X^{q+} + H \rightarrow X^{q+} + H^+ + e$$

and excitation where (n,ℓ) states are specified

$$X^{q+} + H \rightarrow X^{q+} + H(n,\ell)$$

are all of interest.

For H_2 targets we have in addition, dissociative one-electron capture

$$X^{q+} + H_2 \rightarrow X^{(q-1)+} + H^+ + H$$

dissociative single ionization

$$X^{q+} + H_2 \rightarrow X^{q+} + H^+ + H + e$$

two-electron capture

$$X^{q+} + H_2 \rightarrow X^{(q-2)+} + H^+ + H^+$$

transfer ionization

$$X^{q+} + H_2 \rightarrow X^{(q-1)+} + H^+ + H^+ + e$$

(which includes a contribution from autoionizing double capture) and double ionization

$$X^{q+} + H_2 \rightarrow X^{q+} + H^+ + H^+ + 2e$$

For He targets, the processes of two electron capture, double ionization and transfer ionization must be considered together with the above processes for atomic hydrogen.

Ions of Fe, Ni, Ti and Cr are typical of a number of metallic impurity species in fusion plasmas and data are required for charge states ranging from q = 1 to fully stripped at energies from ~ 10 eV u^{-1} to ~ 1 MeV u^{-1}.

2. Total Cross Sections for Electron Capture

Some experimental data are available (see Table 1) for Fe^{q+} ions in H, H_2 and He for q between 3 to 26 at energies within the range 0.01 - 14,262 keV u^{-1} although there are many gaps. For q > 5 and energies below about 25 keV u^{-1} cross sections are only weakly dependent on energy and increase with q. This behaviour is characteristic of partially ionized heavy ions where electron capture takes place through a number of curve crossings[2]. At higher energies where cross sections decrease rapidly with increasing velocity, cross sections for q > 5 scale as q^n where n (typically between 2 and 3) varies slowly with velocity.

Table 1: Experimental Data on Total Electron Capture Cross Sections for Fe^{q+} Ions[1]

Target	Charge State	Energy Range keV u^{-1}	Accuracy	Reference
H, H_2	$3 \leqq q \leqq 14$	0.01 - 0.095	25%	Phaneuf[26]
H, H_2	5,6	0.3 - 2.2	20% H 15% H_2	Crandall et al[27]
H_2	3,5	0.02 - 0.05	?	Huber and Kahlert[28]
H	$4 \leqq q \leqq 13$	27 - 290	35%	Gardner et al[29]
H, H_2	$4 \leqq q \leqq 15$	60 - 161	20% H 15% H_2	Meyer at al[30]
H_2	$11 \leqq q \leqq 22$ 9 12	1,100 277 14,262	15%	Berkner et al[14]
H_2	$3 \leqq q \leqq 13$ $9 \leqq q \leqq 16$ $16 \leqq q \leqq 22$ $20 \leqq q \leqq 25$	103 294 1,160 3,400	20%	Berkner et al[31]
H_2	$20 \leqq q \leqq 25$	3,400	20%	Berkner et al[32]
He	26	7,143	45%	Jolly et al[33]

Phaneuf et al[1] have considered the available experimental and theoretical data for H and H_2 and shown that these can be described in terms of empirical scaling relations using reduced cross sections $\tilde{\sigma} = \sigma/q$ and reduced energy $\tilde{E} = E/q^{1/2}$. The data follow well defined curves over a wide range of reduced energies with an r.m.s. deviation of only 25%. The following form is given for the cross sections $\sigma(q,E)$

$$\sigma(q,E) = \frac{A \ q \ \ell n \ (B\sqrt{q}/E)}{1 + C(E/\sqrt{q})^2 + D(E/\sqrt{q})^{4.5}}$$

where values of the parameters A, B, C and D are tabulated[1]. Recent calculations[3] provide further support of this scaling relation for wide range of charge states in H. Predictions are also given for He (where experimental data are very sparse) with an estimated r.m.s. deviation of 70%.

For Ti^{q+} ions the only experimental data[4] available are for Ti^{2+} ions in H and H_2 at energies ranging from 3-1000 keV with an accuracy of about 10%. Cross sections for the near resonant Ti^{2+} -H process are in good agreement with cross sections for the inverse Ti^{+} -H^{+} process at the same c.m. energies[4].

The only calculations for Ti^{q+} collisions are those for Ti^{4+} +H. The cross sections were predicted for energies from ~ 100 eV u^{-1} to 80 keV u^{-1} using both the molecular orbital[6] and atomic orbital[7] methods. There are also some calculations[6] for Ti^{3+} -H^{+} charge transfer (i.e. the inverse of Ti^{4+} -H).

Although specific data on Ti^{q+}, Cr^{q+} and Ni^{q+} are very limited, a general scaling prediction[8] is available from which total one-electron capture cross sections for species with $q \geqq 5$ may be inferred with an accuracy to within about 50% over a very wide velocity range. It should be emphasised that this generalised scaling does not apply to low charge states $q < 5$.

There are no data for two-electron capture for the species of present interest. However, measurements[9] with many other heavy partially ionized species at energies below about 10 keV amu^{-1} indicate that while cross sections for two-electron capture are generally smaller than those for one-electron caputre, the relative importance of the two-electron capture processes increases with q.

The transfer ionization process in H_2 and He can provide a very important contribution to total electron capture particularly at the lower impact energies[10]. At energies above 50 $q^{1/2}$ keV u^{-1}, ionization will provide the main contribution to the electron removal process.

At low impact energies, for high values of q there are data which suggest that for a helium target, one-electron capture may also favour simultaneous excitation of the target[11].

3. State-Selective Electron Capture

There are no experimental data for the species of present interest. At energies below about 25 keV u^{-1} electron capture by partially ionized species is likely to be influenced by a number of curve crossings which are specific to particular collision systems. General scaling procedures of the type to describe total electron capture cross sections are therefore inappropriate. Experimental data for partially ionized argon[12] ions in H are illustrative of the general pattern. Multi-channel Landau-Zener calculations can often be used to identify the dominant collision channels, but generally do not provide quantitative information of the required accuracy. Much better accuracy can be achieved in quantum mechanical calculations, at least in cases of closed-shell projectile ions, and some calculations are available[6,7] for Ti^{4+}, Cr^{6+} and Fe^{8+} + H collisions.

At energies above about 50 keV u^{-1} CTMC calculations have provided useful data on one-electron capture for carbon and oxygen ions and have been extended to the species of present interest[3,13]. However, for He and H_2 targets, this approach cannot be considered reliable due to the difficulty of describing the competition from two-electron processes.

4. Ionization

There are practically no experimental data for the species of present interest. Limited measurements have been carried out[14] only for Fe^{q+} in H_2 for q between 3 and 59 at energies within the range 0.31 to 4.65 MeV u^{-1}. However, the pattern of ionization in H above 200 keV u^{-1} is well established from measurements[15] with a wide range of ion species. At these high velocities cross sections for ionization at a particular impact velocity increase according to q^n for $q > 5$ where n varies slowly with velocity.

In addition, Gillespie[16] has developed a scaling relation for ions with $q \geqq Z/2$ within the Bethe-Born approximation which provides a good description of the experimental data[15] (even when $q < Z/2$) for a number of different ions ranging from protons to argon and q up to 8 in H for energies $(E/A)/q \geqq 30$ keV u^{-1}. Expressions of the same functional form have also been found to satisfactorily describe the available experimental data for H_2 and He targets.

A general scaling relation for cross sections for electron removal (dominated by ionization above 300 keV amu^{-1}) based on CTMC predictions[3,17] provides an approximate description of available experimental data for q between 1 and 50 and energies between 50 and 1000 keV u^{-1}. Similar σ/q and E/q scalings[18] reduce CTMC results for H_2 and He targets to a common curve for Fe^{q+} and $q \geqq 5$. The scaling is inappropriate for lower values of q.

At energies significantly below the peak in the ionization cross section, experimental data are very sparse and it is therefore difficult to identify the range of validity of theoretical predictions at the present time.

5. Excitation

The data base for hydrogen excitation in X^{q+}-H collisions at energies above some 10 keV u^{-1} q^{-} has been evaluated recently[19] and found to be well described (in the Janev-Presnyakov[20] (σ/q vs. E/q)-scaling representation) by an empirical universal curve due to Lodge et al[21], except at energies below 100 keV u^{-1} q^{-1}. In the energy regime between 10 and 100 keV u^{-1} q^{-1} there are no experimental data except for H^+ projectiles while results from various theoretical assessments for projectiles of higher q diverge considerably. These results together with some new theoretical predictions[7,22] indicate that low-energy excitation cross sections do not obey Janev-Presnyakov scaling and hence deviate greatly from the curve due to Lodge et al.

Excitation cross sections in X^{q+} -He collisions have been measured[23-25] for a number of projectile states and a selection of final excited He states. Their general behaviour is very similar to the case of excitation of atomic hydrogen. Approximate scaling of these cross sections with charge q has been demonstrated recently[23]. This is the case particularly for the optically allowed transitions cross sections for $q > 1$ from measurements[24,25] for proton impact. The scaling relation deteriorates at energies below some 50 keV u^{-1} q^{-1} and is not considered valid below 25 keV u^{-1} q^{-1}.

6. Conclusions

Although specific data on collision processes involving Fe, Ni, Ti and Cr ions in H, H_2 and He are sparse, general scaling relations should allow the prediction (with an accuracy generally within 50%) of total one-electron capture cross sections and ionization cross sections for initial charge states $q \geqq 5$ over a wide velocity range. There is also evidence that scaling relations may also be applied to collisions involving excitation. However for low impact velocities and for ions of low q where these scaling procedures are generally invalid, specific measurements and calculations are required.

In the case of state selective electron capture where scaling procedures are invalid there is an urgent need for reliable data on each collision combination. In experiments where metastable as well as ground state primary ions are often present, it is essential to avoid ambiguities in interpretation. Cross sections specific to ground and metastable primary species are required.

Data for excited target species (especially H) are required. At present there are very few measurements or calculations for any primary ion species.

Data for charge transfer and ionization in ion-ion collisions would be of interest. While collisions of both singly and multiply ionized metallic ions with protons are of relevance, collisions with He ions are also important in the context of alpha particle heating.

There are a number of laboratories with well established programmes which might contribute to an improved database. Further experimental measurements would appear to within the capacity of the groups in Belfast (Gilbody), Oak Ridge (Phaneuf), Groningen/Amsterdam (Morgenstern and de Heer), Aarhus (Anderson and Hvelplund), Stockholm (Barany), Tokyo (Kaneko), Giessen (Salzborn) and Leningrad (Afrosimov). Further calculations seem appropriate to the interests of the groups in Rolla-Missouri (Olson), Berlin (Fritsch), Belfast (Crothers), Moscow (Presnyakov), Paris (McCarroll), Paris (Katsonis), Rosario (Rivarola), Aarhus (Taulbjerg), Durham (Bransden, Ermolaev), Argonne (Kimura) and Kansas State (Shingal, Lin).

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4. MEETING CONCLUSIONS AND RECOMMENDATIONS

The participants adopted the conclusions of the Working Group regarding the data status and the data quality formulated in their Reports (Section 3). Some general conclusions can be drawn from the analysis performed by the Working Groups:

1) The database for the electron-impact processes of the considered metallic ions is still rather incomplete, either in terms of availability or required accuracy. More experimental data (particularly for excitation and RR) are urgently needed to validate the theoretical models.

2) The database for the heavy-particle collisions of the considered species is also in an unsatisfactory state (except for the total single-electron capture cross section for $q \geqq 5$). More extensive work, both theoretical and experimental, is needed in the areas of state-selective electron capture, excitation, dissociative processes in ion collisions with H_2 and on processes involving excited target states.

3) The role of metastable states in both electron-ion and ion-atom (molecule) collisions needs careful clarification before the interpretation of experimental data is proposed.

In view of the unsatisfactory situation in the database for metallic impurities in fusion plasmas, and having in mind the growing needs for such data in the present fusion research and reactor design work, the Meeting participants have made the following recommendations to the IAEA Director General and the IAEA Atomic and Molecular Data Unit:

1) To initiate as soon as possible a Co-ordinated Research Programme, with inclusion of the world most active theoretical and experimental groups and laboratories for the generation of the required A+M database on fusion plasma metallic impurities in a co-ordinated fashion. The participants in this CRP should have sufficiently high expertise for a competent assessment of the quality of generated data, both within and outside the CRP.

2) The scope of the recommended CRP should also include metallic impurities related to materials which are of current fusion interest, or considered as candidate materials for the plasma facing components of next-step fusion reactors (e.g. Be, Al, Mo, W).

3) To organize a systematic compilation and evaluation of the metallic impurity data within the IAEA A+M Data Unit and through the A+M Data Centre Network. This activity should be appropriately related with the activity of the above proposed CRP.

The Meeting participants also supported the idea to publish the contributions to the meeting and the Working Group Reports in a Topical Issue of "Physica Scripta".

Appendix 1

IAEA Advisory Group Meeting on "A+M Data for Metallic Impurities in Fusion Plasmas"

Vienna, 16-18 May 1990
Vienna International Centre, Vienna, Austria

Scientific Secretary: Dr. R.K. Janev, RIPC

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Appendix 2

IAEA Advisory Group Meeting on "A+M Data for Metallic Impurities in Fusion Plasmas"

May 16-18, 1990, Vienna, Austria

MEETING AGENDA

Wednesday, May 16 (Meeting Room: C-07-IV)

9:30 - 9:45 Opening

Section 1: Electron-ion collisions: Recombination
Chairman: V. Abramov

9:45 - 10:30 Y. Hahn: Radiative and dielectronic recombination of electrons on Ti, Cr, Fe and Ni ions

10:30 - 11:00 N. Badnell: Density effects in dielectronic recombination

11:00 - 11:15 Coffee break

11:15 - 11:50 M. Bitter: Measurements of dielectronic recombination rate coefficients for He-like and H-like metal ions from tokamak plasmas

11:50 - 12:20 A. Müller: Radiative recombination of free electrons with ions

12:20 - 14:00 Lunch

Section 2: Electron-ion collisions: Excitation and Ionization
Chairman: Y. Hahn

14:00 - 14:30 D. Gregory: Electron-impact excitation of metal ions

14:30 - 14:45 R. Clark, J. Abdallah: Excitation and ionization of Ti ions (will be presented by D. Gregory)

14:45 - 15:15 V. Shevelko: CBE calculations of electron-impact excitation of Ti^{q+}, Cr^{q+} and Ni^{q+} ions

15:15 - 15:45 K. Berrington: Electron collision R-matrix calculations in progress at Queen's University of Belfast

15:45 - 16:00 Coffee break

16:00 - 16:30 A. Müller: Electron-impact ionization of ions

16:30 - 17:00 N. Badnell: Ionization cross sections and rate coefficients for transition metal ions

17:00 - 17:30 S. Younger: (pending) (will be presented by N. Badnell)

17:30 - 18:00 V. Shevelko: Born-Oppenheimer calculations of electron-impact ionization of Ti^{q+}, Cr^{q+} and Ni^{q+} ions

18:00 - 18:30 V. Abramov: Comparison of the existing evaluated A+M data for fusion

19:30 - Joint Dinner

Thursday, May 17 (Meeting Room: C-07-IV)

Section 3: Heavy-particle collision: Experimental and quantum-mechanical results

Chairman: R. Olson

9:00 - 9:45 H. Gilbody: Measurements of cross sections for charge exchange, state selective capture and ionization by metallic ions

9:45 - 10:30 W. Fritsch: Theoretical investigations of electron transfer from atomic hydrogen to closed 3n-shell ions of Ti, Cr and Fe.

10:30 - 10:45 Coffee break

10:45 - 11:20 G. Yudin: The unitary semiclassical theory of coulomb excitation of atoms

11:20 - 12:00 H. Cederquist: Collisions of very highly charged ions with atoms

12:00 - 14:00 Lunch

Section 4: Heavy-particle collisions: CTMC results

Chairman: H. Gilbody

14:00 - 14:45 R. Olson: Electron removal cross sections for H, He and H_2 by metallic impurity ions at 0.1 - 1.0 MeV/u

14:45 - 15:30 K. Katsonis: CTMC cross sections for ionization and electron capture in collisions of multicharged ions with atomic hydrogen

15:30 - 16:00 Coffee break

Section 5: General discussion of atomic database for metallic impurity ions

Chairman R. Janev

16:00 - 18:00 - Discussion of the status and quality of atomic database for metallic impurities,

- Co-ordination of future data production and evaluation activities,
- Formation of data evaluation Working Groups for:

  a) Electron-impact collision data,
  b) Heavy-particle collision data.

Friday, May 18

Section 6: Data evaluation and preparation of Working Group Reports (work in parallel sessions)

9:00 - 12:00	Working Group on Electron-impact processes (Room: A-0715)	Working Group on Heavy-particle collisions (Room: C-07-IV)
12:00 - 14:00	Lunch	

Section 7: Discussion of Working Group Reports and Adoption of AGM Recommendations (Room: C-07-IV)
Chairman: R.K. Janev

14:00 - 15:00	Discussion of Working Group Reports
15:00 - 15:30	Preparation of Meeting Recommendations
15:30 - 16:00	Coffee break
16:00 - 17:00	- Adoption of Working Group Reports and Meeting Recommendations - Publication of Meeting Proceedings