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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

3rd IAEA Research Co-ordination Meeting on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling"

March 8-9, 1999, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared by: R.K. Janev

April, 1999

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

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Abstract

A brief description of the proceedings and the conclusions of the 3rd Research Co-ordination Meeting on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling", held on March 8-9, 1999, at the IAEA Headquarters in Vienna, Austria, is provided. The reports on the activities within the individual projects pertinent to the IAEA Co-ordinated Research Program with the same title are given as appendix to the present report.

Reproduced by the IAEA in Austria
April, 1999

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1. INTRODUCTION

The 3rd Research Co-ordination Meeting of the participants of the IAEA Co-ordinated Research Project (CRP) on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling" was held on March 8-9, 1999, at the IAEA Headquarters in Vienna, Austria. The objectives of the meeting were:

a) to review the results of the work done within the individual CRP projects in the period between the 2nd and 3rd RCM;
b) to summarize the overall accomplishments of the CRP in the entire previous period of its activity;
c) to co-ordinate the research programmes for the remaining period of CRP activity (end of year 2000);
d) to define and agree on the format of the joint publication resulting from the CRP.

The meeting was attended by the principal scientific investigators of the individual CRP projects, except for Prof. G. Billing, Prof. T. Fujimoto and Prof. K. Snowdon who were not able to attend. Prof. V. Ferleger attended the meeting in lieu of Prof. U. Rasulev. The List of Meeting Participants is given in Appendix 1.

2. BRIEF MEETING PROCEEDINGS

After the welcome address of the Scientific Secretary of the Meeting (R.K. Janev) and the adoption of Meeting Agenda (see Appendix 2), the meeting continued its work in five consecutive sessions.

The first session of the meeting (chaired by F. Brouillard) was devoted to electron-impact processes taking place in divertor plasmas. The first speaker of this session, Prof. T. Märk reported on the recent work done by his group on electron-impact ionization (and some other) processes of edge plasma constituents. The experimental methods for cross section (total and differential) measurements were described and representative results for selected collision systems were shown. The ionization processes studied included single and multiple e-impact ionization of atoms, molecules and molecular ions, and e-impact dissociation of molecular ions. Besides the total cross sections, the energy distribution of reaction products was measured in these experiments. The atomic and molecular species included in these studies where those having direct relevance to the fusion edge plasma research (species containing H, He, C, N, O in atomic or molecular (molecural ion) form). In addition, Prof. Märk presented the physical basis of their originally developed semi-empirical model for calculation of single and multiple e-impact ionization of atoms, ions, molecules and clusters, and demonstrated its applicability and efficiency (accuracy) on a number of collision systems.

The second speaker in this session was Prof. J.M. Wadehra who reported on his group's recent cross section calculations for the processes of dissociative electron attachment and resonant dissociation of vibrationally excited isotopic hydrogen molecules by electron impact. The results of a large number of cross section calculations (for several isotopic systems in all available vibrationally excited states) were presented. Prof. Wadehra also showed the results of his derivations of the cross section scaling relations (with respect to the initial vibrational quantum number and the isotopic mass ratio). A closed form expression was shown also for the rate coefficient of dissociative electron attachment which successfully approximates the numerical results.

Prof. M. Capitelli provided a comprehensive review of the recent results obtained by his group on (i) e-impact excitation and ionization cross section calculations for a variety of vibrationally excited isotopic hydrogen molecules, (ii) kinetics calculations in hydrogen plasmas involving all important processes and species, and (iii) a number of processes in the interaction of isotopic hydrogen molecules with solid surfaces. This information is highly important for the construction of a complete collisional-radiative model for the $H_2(v)/H$ system and, in general, for a complete description of neutral hydrogen behaviour in the edge plasma, including the effects of particle-surface interaction processes.

The last speaker in this session was Prof. F. Brouillard, who reported on the recent experimental cross section measurements for electron-impact single and multiple ionization of some (Ni) multiply charged ions, and on the e-impact ionization and dissociation of a number of molecular ions (N_2^+, O_2^+, CO_2^+, H_2O^+, H_3O^+, and isotopic variants) performed in his Laboratory (by the group of Dr. P. Defrance). The experimental methods for these measurements were also described. Prof. Brouillard discussed the underlying physics of the studied processes to explain certain characteristic features of the measured cross sections.

The second session of the meeting was devoted to heavy-particle collision processes and was chaired by Prof. T. Märk. The first speaker in this session was Prof. C. Harel who presented the results of the extensive calculations of his group on electron capture processes in slow collisions of C^{4+} with H and H_2. The MO close-coupling method was employed in these calculations, with appropriate care being taken to describe the two-electron situation in C^{4+} and H_2 (as well as the ro-vibrational motion in H_2). The results of the calculations (with various basis sets, including pseudo-states, and various model potential approximations) were compared with the calculations of other authors and with the experimental results.

The second speaker in this session was Prof. E.A. Solov'ev who reported on certain analytical derivations for the electron momentum distribution of ejected electrons in slow ionizing collisions of a bare ion with a one-electron atomic system. The derivations were based on the so-called S-superpromotion mechanism for "direct" ionization which comes out from the "hidden crossings" description of collisional dynamics in the adiabatic energy region. No specific numerical calculations were provided however.

Prof. H. Tawara reported on the results of cross section calculations of several Japanese research groups for the processes of vibrational excitation, electron capture and particle exchange in slow collisions of ions, atoms and molecules with ro-vibrationally excited molecules, all species being hydrogenic (including isotopic variants). (Helium was also included among the atomic species). The calculated cross sections for a large number of collision systems were shown, allowing to derive some general conclusions for the cross section dependence on the initial rotational and/or vibrational quantum number. Of particular importance are the results on the proton-molecular hydrogen (vibrationally excited) charge exchange reaction which plays an important role in the volume plasma recombination in the divertor region.

The last speaker in this session was Prof. F. Brouillard who presented the results of cross section measurements for the processes of mutual neutralization, transfer ionization and associative detachment in slow collisions of H^- and D^- with a number of atomic and molecular ions (involving H^+, He^+, H_2^+ / D_2^+, C^+ , N^+ , O^+). He also presented the cross section measurements results for the associative ionization in slow atom-excited atom collisions (involving isotopic hydrogen species). Both the applied experimental methods and the underlying physics of these processes were adequately described. Prof. Brouillard also discussed some scaling relationships for the studied processes.

The third session of the meeting (chaired by Prof. H. Tawara) was devoted to particle-surface interaction processes. The first speaker in this session was Prof. T. Märk who presented an extensive account on the surface induced reactions of edge plasma constituents. Prof. Märk first described the characterics of their experimental set-up BESTOF and the experimental methodology. The results of the studies of fragmentation processes of a number of hydrocarbon and other polyatomic (e.g. $C_n H_m O_p$) ions interacting with selected surfaces were shown and analyzed in the context of hydrogen recycling in divertors. The second speaker in this session was Prof. V. Ferleger. He presented the recent results obtained in his Institute (Arifov Institute of Electronics, Tashkent) on electron-impact induced sputtering (measurements of positive yield), secondary electron and ion emission induced by multicharged ion impact on surfaces (experimental and theoretical studies), measurements of the ionization degree of single-scattered noble gas atoms from various surfaces, including theoretical studies for the processes of multicharged ion-impact on surfaces (ion emission, scattering of hyperthermal rare gas atoms, etc). The presentation provided a clear picture of the underlying physics for most of the studied processes, supplemented in many cases with a relatively simple theoretical model.

The last two sessions of the meeting (chaired by R.K. Janev) were devoted to a summary of the CRP results achieved so far, discussion of the work co-ordination within the CRP untill its formal termination (end of year 2000) and to the method of preparation and the format of the CRP joint publication, resulting from the CRP work. The results of the discussions and the

conclusions of these two sessions are summarized in the next two sections of the present report.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

The assessment of the overall success of the CRP in achieving its objectives was done on the basis of brief reports of the meeting participants for the activities within each CRP project for the entire duration of the CRP. These reports are reproduced in Appendix 3 (some of them being submitted after the meeting). Both the discussion at the meeting and the activity reports in Appendix 3 (each being supplemented by a list of relevant publications for the period covering the CRP duration) demonstrate that the CRP has already (i.e. more than one year before its termination) achieved its basic objective: to significantly increase the quantitative atomic and particle-surface information required for modeling of fusion reactor divertor plasmas. On average, about twenty publications have been published by each of the participating CRP groups within the scope of their CRP projects (with a singularity of 121 publications by the group of Prof. T. Märk). The CRP effort has produced very important data contributions in the fields of electron-impact processes (all types) involving vibrationally excited hydrogen isotope molecules and ground state impurity molecules and molecular ions, (including hydrocarbons), electron-atom (ion) collision processes, heavy-particle collision processes (involving ions, atoms (also in excited states), molecules and molecular ions), particle (electron, ion, atom, molecule, molecular ion)-surface collision processes (involving a large spectrum of processes) and the construction of the collisional-radiative model for H_2/H system. As a result of the numerous data obtained by the present CRP, the divertor modeling computer codes can now include the vibrational and electronic excited state kinetics, electron rearrangement and ion conversion kinetics and the plasma wall interaction kinetics. These three physics areas were either very modestly included or completely absent in the existing codes for divertor plasma modeling.

Despite of the significant amount of new quantitative information produced by the CRP on the collision processes involved in the divertor plasma, including particle-surface interaction processes, there are still important classes of processes or collision systems for which the degree of completeness of the required database is still not satisfactory. This is particularly true for the processes involving hydrocarbon molecules (and other carbon and oxygen containing molecules) and the particle-surface interaction processes and reactions. The data defficiency in the latter case is especially pronounced for material surfaces of current fusion interest (Be, C and W) and is partly caused by the large variety of possible processes which can take place during the interaction of plasma and impurity particles with the surfaces.

Based on the above assessments and other discussions, the meeting participants have come to the following conclusions and recommendations:

1) The present CRP has produced a significant amount of new atomic and plasma-wall interaction data to considerably improve the physics basis of the divertor plasma modeling codes;
2) In the remaining period of the CRP duration (end of year 2000), additional data relevant to divertor plasma modeling will be generated by the CRP participants;
3) An important task for the CRP participants in the remaining period of CRP duration is to collect and appropriately format the data generated within the individual CRP projects (as well as some other relevant data generated in non-CRP laboratories);
4) In order to fulfill this task, the RCM participants have agreed to write one or two review papers (25-40 pages each) on the subject of their CRP project, where the data generated (and published) within their laboratories during (and even before) the CRP would be presented, including also important data from other laboratories;
5) The collection of these reviews will be published as a separate volume of the IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion" during the year 2000. The deadline for submission of the manuscripts is the end of January 2000.
6) The manuscripts should be prepared in a camera-ready form; the format and manuscript preparation instructions are given in the following section of the present Summary Report;
7) In view of the fact that there are still significant defficiencies and gaps in the database for particle-surface interaction processes, particularly for material surfaces of prime fusion interest, the RCM participants recommend to the IAEA to include in its programme planning for the years beyond 2001 two separate CRPs.
    1) Particle-surface interaction processes in fusion reactor divertors; and
    2) Collision processes involving edge plasma molecular impurities.
8) It is, further, strongly recommended that Dr. R.K. Janev is included as participant to the present CRP after the termination of his current contract with the IAEA.

4. FORMAT OF THE CRP JOINT PUBLICATION

The manuscripts for the above mentioned joint publication resulting from the CRP should be prepared in a camera-ready form. The style is, generally, that of the Nuclear Fusion journal, with the important difference that the text is on the entire page (not in two columns). The text starts 2.5 cm from the top of the (A-4) page, it is 17 cm and 23 cm in the horizontal and vertical dimension, respectively.

The title is in bold capitals (fonts Times New Roman, size 12 pitch). All other text is in fonts Times New Roman, size 12 pitch, with one interline spacing. The author name(s) is(are) also in Capital letters (not bold), as are the titles of sections (numbered by arabic numerals). Titles of tables (numbered by roman numerals) are also in capitals and placed above the table. Figure captions are in italic. All tables and figures should be embedded in the proper place in the text. References in the text are in squared brackets. An Abstract preceeds the main text starting with 1. INTRODUCTION. All this is illustrated on the attached sample pages p.11

and p.12. The titles of sub-sections and sub-sub-sections are written in a normal way but in bold, as illustrated on p.13. Page 14 gives the model for making the reference list at the end of the text. (Note that the volume number is in bold).

The manuscripts in the above described format and style can also be submitted electronically in PostScript to the e-mail address: j.stephens@iaea.org or: jsteph@ripcrs01.iaea.or.at

THEORETICAL STUDIES ON SLOW COLLISIONS BETWEEN MEDIUM-Z METALLIC IONS AND NEUTRAL H, H_2, OR He

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Abstract

The database on electronic transitions in slow collisions between medium-Z metallic ions and H, H_2, and He targets is examined. Semiclassical close-coupling calculations are presented for electron transfer in Si^{4+}–H, Ni^{10+}–H, Si^{4+}–He, Ti^{4+}–He, Ti^{4+}–H_2, and Fe^{8+}–H_2 collisions in an energy range of about 1 – 100 keV/u. The calculated distributions of electron transfer over the final states of the projectiles are discussed. For the case of Si^{4+}– He collisions, we also assess the process of target excitation.

1. INTRODUCTION

In the past 15 years there has been considerable progress in the understanding and description of atomic collisions at low and intermediate energies where perturbation theories do not apply. Close-coupling schemes have been devised with increasing complexity, in order to account for the many transitions which are populated in such collisions [1, 2, 3]. Among specific areas of progress we mention the ability to describe *weak transitions* to final states which are far off resonance with the initial state, the description of *two-electron transitions* in ion-atom collisions, and the description of ion-*molecule* collisions. Naturally, in these very areas there are still limitations of present implementations of the close-coupling method, due to the complexity of the required numerics or in some cases due to conceptual problems.

Much of this progress has been motivated by the curiosity of basic research *and* by the needs of applied research at fusion plasma facilities. The need for detailed cross sections, including notably the distribution of transitions over final states, in collisions between metallic ions and basic plasma constituents is a challenge for both theory and experiment which, at low energies, can only be met for selected systems. At those energies, each system behaves differently according to its two-center quasi-molecular structure so that only the *total transfer* cross section can be related directly from equi-charged systems. There has been theoretical work in the past, that has concentrated on specific systems which are of interest here, like an investigation of electron transfer in Si^{q+}–H systems (q=4...14) [4] and an investigation of collisions between the closed-3p-shell ions of Ti, Cr, and Fe with atomic hydrogen [5]. These studies are the only ones that have determined partial transfer cross sections. For energies above 10 keV/u, total transfer cross sections have been determined for a set of Ti^{q+}, Cr^{q+}, Fe^{q+} and Ni^{q+}– H systems within the classical-trajectory-Monte-Carlo method [6]. No experimental data exists to date on the final-state population in slow collisions. There is also no data on target excitation in these systems. A short review of the data base for collisions between metallic impurity ions with H, H_2, and He, as of 1991, has been published [7]. A recent update to this report is also available [8].

In this work we present an investigation on a set of six low-energy collision systems. Earlier work on the Si^{4+}–H system [4] is extended in energy and augmented by considering a He target. Our work on closed-3p-shell metallic projectiles [5] is extended by including the Ni^{10+} projectile and also the Ti^{4+}–He system. Out of the class of collisions with H_2 targets we study the systems with Ti^{4+} and Fe^{8+} projectiles. All these studies are examples of what can be done theoretically for systems which have a well-defined atomic structure in the projectile. Systems with a complex multi-particle atomic structure in the projectile are less suitable for investigations by either theory or experiment, they are hence also less suitable for the purpose of plasma diagnosis at fusion devices. On the other hand, *total* transfer cross sections can be predicted for all these system, with much

for q = 3 and 4 at energies of q×2 and q×4 keV. The interpretation of these measurements is complicated by the presence of unknown fractions of metastable ions in the primary beams used. An indication of the likely relative importance of these metastable states is provided by the statistical weights shown in Table 1. However, the lifetimes of these states are unknown so it was not possible to determine the extent to which decay would occur during transit of the ion beams from source to target.

TABLE I. ENERGIES AND STATISTICAL WEIGHTS OF Fe^{3+} AND Fe^{4+} GROUND AND METASTABLE STATES.

State	Energy above ground state (eV)	Statistical Weight (%)
$Fe^{3+}(3d^5)^6S$	0.0	4
^4G	4.0	44
^4P	4.4	
^2I	5.8	
^2D	6.1	30
^2S	8.3	
$(3d^4 4s)^6D$	15.9	22
$Fe^{4+}(3d^4)^5D$	0.0	62
^3P	3.1	19
^1G	4.5	19

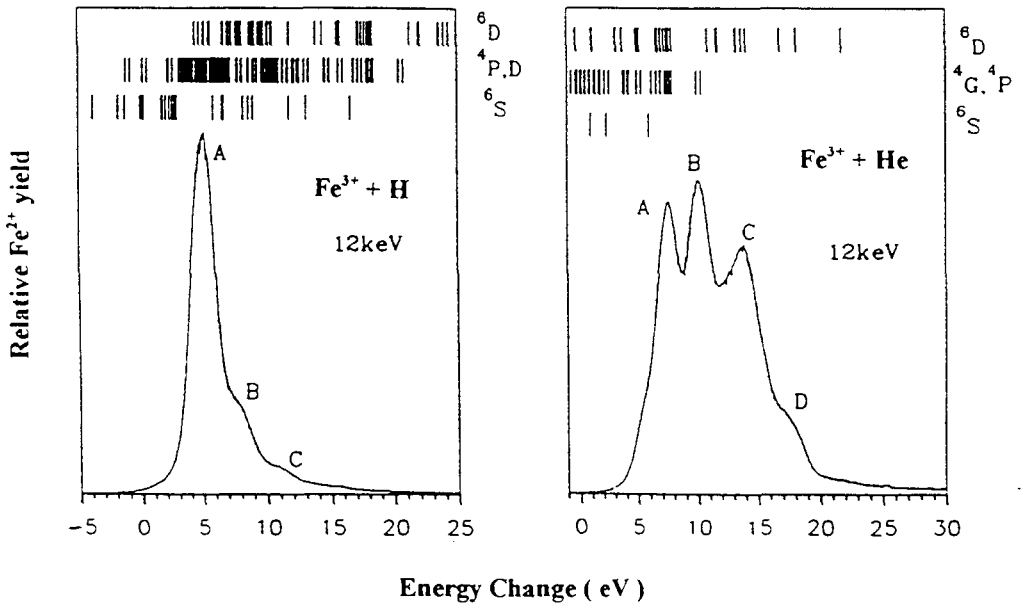

Figure 2. Energy change spectra for one-electron capture in 12 keV Fe^{3+}-H and Fe^{3+}-He collisions. Energy defects corresponding to possible collision product channels involving the ^6S ground state and ^4G, ^4P and ^6D metastable primary Fe^{3+} ions are indicated. (from [5])

3. RESULTS OF THE CALCULATIONS

3.1. Collisions with atomic hydrogen

3.1.1. Si^{4+}– H collisions

Previous work on Si^{q+}– H collisions [4] is extended, for the Si^{4+} projectile, in a number of ways. The energy range is enlarged to include 0.2 – 100 keV/u. The n=6 capture states are included at the projectile in order to improve the accuracy of the calculated transfer cross section to n=5 states. At the hydrogen center, we include the n=2 states of hydrogen. Except for these changes, we keep closely to the prescriptions of the calculations in ref. [4]. The calculated partial transfer cross sections are given in Table I. The results of the calculations are summarized in figure 1.

energy	n	s	p	d	f	g
0.2	3	2.37E-18	1.36E-17	2.61E-15		
	4	7.21E-16	4.47E-17	1.21E-16	1.69E-18	
	5	2.10E-17	7.75E-17	5.61E-18	5.49E-17	1.42E-17
0.3	3	3.31E-18	1.77E-17	2.74E-15		
	4	5.92E-16	4.83E-17	1.08E-16	2.20E-18	
	5	5.41E-17	7.40E-17	7.54E-18	4.40E-17	2.42E-17
0.5	3	1.89E-18	3.86E-17	2.32E-15		
	4	5.86E-16	7.78E-17	1.37E-16	9.45E-18	
	5	1.27E-16	6.06E-17	2.27E-17	3.07E-17	2.90E-17
1	3	4.47E-18	1.23E-16	1.98E-15		
	4	5.16E-16	8.36E-17	1.19E-16	2.12E-17	
	5	9.46E-17	4.32E-17	1.95E-17	2.44E-17	2.50E-17
2	3	1.39E-17	2.99E-16	2.04E-15		
	4	4.20E-16	9.26E-17	9.52E-17	3.18E-17	
	5	4.16E-17	3.00E-17	2.73E-17	3.72E-17	5.86E-17
4	3	2.52E-17	4.72E-16	1.74E-15		
	4	3.89E-16	1.35E-16	9.42E-17	7.84E-17	
	5	2.54E-17	3.18E-17	4.61E-17	4.63E-17	4.63E-17
8	3	2.20E-16	4.87E-16	1.15E-15		
	4	2.80E-16	2.34E-16	7.27E-17	1.27E-16	
	5	9.60E-18	1.29E-17	2.07E-17	2.07E-17	1.26E-17
15	3	1.47E-16	4.15E-16	7.63E-16		
	4	1.16E-16	2.49E-16	1.20E-16	4.23E-16	
	5	1.06E-17	2.78E-17	2.43E-17	2.22E-17	4.35E-17
25	3	1.08E-16	3.53E-16	5.45E-16		
	4	4.56E-17	1.46E-16	1.09E-16	5.24E-16	
	5	8.79E-18	4.05E-17	4.50E-17	1.04E-16	3.02E-17
40	3	6.71E-17	2.55E-16	4.16E-16		
	4	1.69E-17	7.71E-17	1.07E-16	2.90E-16	
	5	7.94E-18	3.15E-17	5.00E-17	1.24E-16	2.98E-17
70	3	1.42E-17	7.83E-17	1.65E-16		
	4	7.99E-18	3.62E-17	7.70E-17	5.80E-17	
	5	6.00E-18	2.14E-17	4.59E-17	3.74E-17	9.29E-18
100	3	3.56E-18	2.16E-17	6.38E-17		
	4	3.27E-18	1.27E-17	3.76E-17	1.47E-17	
	5	2.88E-18	9.03E-18	2.55E-17	1.08E-17	2.39E-18

TABLE I: PARTIAL TRANSFER CROSS SECTIONS TO Si^{3+} $n\ell$ STATES IN Si^{4+}– H COLLISIONS.

As noted and explained in the previous investigation [4], the capture cross section is seen to be dominated

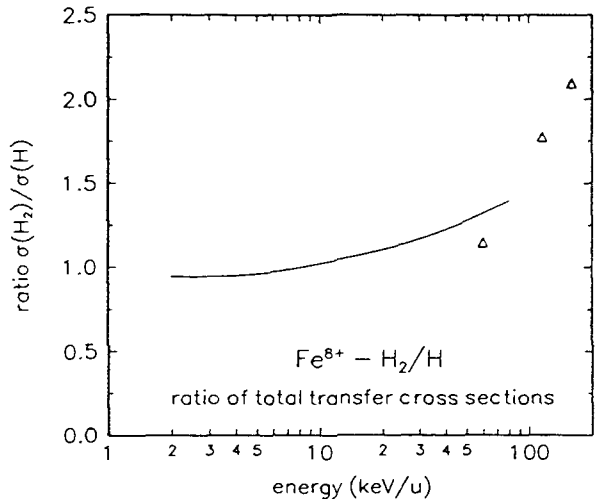

Figure
~~FIG.~~ *10: Ratio of calculated total transfer cross sections for the Fe^{8+}– H_2 system (this work) and the Fe^{8+}– H system [5]. Data are by Meyer et al. [14] (Δ).*

shell. The n distribution of electron transfer should be reliable except for the highest n shell considered in a given study. The ℓ distribution within a given n shell will become less reliable for the higher n shells.

The studies performed in this work are examples of what can be done for other systems of interest if the need arises. There are however clear limitations on which systems can be pursued in a feasible and meaningful manner. The existence of an easy level structure in the charge transfer system is prerequisite for the theoretical description and the use in plasma diagnostics alike. Hence charge transfer systems with only one electron outside an inert core have been considered here. A second electron has been alowed for in the target, in the case of collisions with helium or molecular hydrogen targets. One could also treat systems with a second electron in the projectile ion in a similar way. All slowly colliding systems must be treated in a case-by-case fashion. On the other hand, we have indicated that the n distribution may be interpolated between equi-charged systems if the charge state is sufficiently high.

This work has been performed within an IAEA Co-ordinated Research Project (CRP) on "Atomic Data for Medium- and High-Z Impurities in Fusion Plasmas" (1991-1994). The author is indebted to R.K. Janev for his guidance during all phases of this project, and to him and the other participants for the open exchange of results and ideas at the CRP meeting.

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APPENDIX 1

3rd IAEA Research Co-ordination Meeting on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modelling"

March 8-9, 1999, IAEA Headquarters, Vienna, Austria

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APPENDIX 2

3rd IAEA Research Co-ordination Meeting on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling"

March 8-9, 1999, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, March 8 — **Meeting Room: A-19-72**

09:30 - 09:45	- Opening - Adoption of Agenda	
Session 1:	*Electron Impact Processes*	
Chairman:	**F. Brouillard**	
09:45 - 10:15	T. Märk	Electron impact ionization of edge plasma constituents
10:15 - 10:45	J. Wadehra:	Dissociative attachment and dissociation of molecular hydrogen and its isotopes by electron impact
10:45 - 11:15	*Coffee break*	
11:15 - 11:45	M. Capitelli:	Recent advances in the physics of molecular H_2/D_2 plasmas
11:45 - 12:15	F. Brouillard:	Some recent measurements of electron impact ionization and dissociation cross sections
12:15 - 14:00	*Lunch*	
Session 2:	*Heavy Particle Collision Processes*	
Chairman:	**T. Märk**	
14:00 - 14:30	C. Harel:	Charge exchange in C^{4+} - H, H_2 collisions: comparison between "ab initio" and model potential calculations
14:30 - 15:00	E. Solov'ev:	Electron momentum distribution for direct ionization in slow ion-atom collisions
15:00 - 15:30	*Coffee break*	
15:30 - 16:00	H. Tawara:	Dependence of the cross sections for non-reactive reaction, atom exchange and dissociation on vibrational state in H_2^+ (v) + He slow collisions
16:00 - 16:30	F. Brouillard:	Low energy rearrangement processes involving H^* and H^-: some recent results

Tuesday, March 9 **Meeting Room: A-19-72**

Session 3: *Surface Collision Processes*

Chairman: H. Tawara

09:30 - 10:00	T. Märk:	Surface induced reactions of edge plasma constitutents
10:00 - 10:30	V. Ferleger:	Some peculiarities of inelastic particle-surface interaction in the low-energy range
10:30 - 11:00	*Coffee break*	

Session 4: *Summary of the CRP results*

Chairman: R.K. Janev

11:00 - 12:00 General discussion

12:00 - 14:00 *Lunch*

Session 5: *Form of Publication of Final CRP Outcome; Meeting Conclusions*

Chairman: R.K. Janev

14:00 - 15:30
- Discussion on the form of publication of the CRP outcome;
- Method of preparation of the final CRP product.
(All participants)

15:30 - 16:00 *Coffee break*

16:00 - 17:00 Meeting Conclusions and Recommendations

17:00 - *Adjournment of the Meeting*

APPENDIX 3

3rd IAEA Research Co-ordination Meeting on "Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling"

March 8-9, 1999, IAEA Headquarters, Vienna, Austria

Brief Activity Reports for the Individual CRP Projects

Dissociative attachment and dissociation of molecular hydrogen and its heavier isotopes by electron impact

Contribution to IAEA-CRP (*"Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modelling"*) by **J. M. Wadehra** of Wayne State University.

In the resonance model, the physics of the process of dissociative electron attachment to a molecule AB is described via the formation of a temporary bound state of the electron-molecule system. The electron in this molecular anion state AB^- (also called the resonance state) can autodetach with a finite lifetime (related to the width, Γ, of the resonance), leaving behind a vibrationally excited neutral molecule. On the other hand, if the lifetime of the resonance is long enough, the anion AB^- can dissociate into $A + B^-$, leading to the process of dissociative electron attachment. Thus, in a schematic sense one has

$$e_i + AB(v_i) \rightarrow AB^- \begin{cases} \rightarrow A + B^- \\ \rightarrow e_f + AB(v_f) \end{cases}$$

The final level with quantum number v_f can be either discrete (corresponding to vibrational excitation of the molecule) or could lie in the continuum (corresponding to dissociation of the molecule).

A possible scenario of the resonance model is depicted in .Figure 1. Shown schematically in this Figure are the potential curves of the neutral molecule AB (labeled V_0) and of the resonant state AB^- (labeled V^-). The two potential curves cross at an internuclear separation $R = R_s$ such that, for $R \geq R_s$, the autodetachment of the electron is energetically not permitted and the resonance turns into a stable bound state of AB^-. R_s is referred to as the stabilization radius. Before the incident electron, with energy ε, is captured, the nuclei are vibrating in the level (v_i) under the influence of the potential $V_0(R)$. After electron capture, the nuclei of the anion move under the influence of $V^-(R)$. The probability of electron capture to form the resonant molecular anion state depends on the internuclear separation and this probability is maximum at an internuclear separation (labeled R_c in the Figure and referred to as the capture radius) at which

the energy separation between the two potential curves is equal to the energy of the incident electron. If the potential curve V^- is repulsive in nature, the nuclei in the anion state begin to separate such that the electronic potential energy is converted into nuclear kinetic energy. Now, if the autodetachment of the electron occurs at some specific internuclear separation, labeled R in the Figure, the neutral molecule is left in a vibrationally excited level due to the gain in the nuclear kinetic energy (indicated by a vertical dotted line in the Figure). The exact vibrationally excited level (v_f) achieved by the molecule depends on the gain in the kinetic energy of the nuclei as well as on the relevant selection rules. Depending upon the lifetime of the resonance the nuclei in the anion state may separate to an internuclear separation larger than R_s beyond which the autodetachment of the electron is energetically not possible and dissociative attachment may occur resulting in the formation of a stable negative ion.

A few salient features of the resonance model are worth mentioning. First, the processes of dissociative electron attachment and of vibrational excitation by electron impact are treated on an equal footing so that the investigation of one of these processes leads, in a natural way, to the information related to the other process. In fact, the optical theorem (which essentially is a conservation of flux statement) relates the cross sections for these two processes within the resonance model. Also, it is tacitly assumed that the transition between the resonant state and the electronic state of the neutral molecule is a spontaneous one without any corresponding change in the nuclear positions or velocities (a Franck-Condon transition). This *local* description of the resonance model is valid when the energy of the incident electron is much larger than the spacing of vibrational levels or when the incident electron energy is much above the threshold energy. When the incident electron energy is sufficiently small such that these conditions are not met, a proper description of the resonance model is a *nonlocal* one involving, in its mathematical formulation, an integrodifferential equation with nonlocal complex potential.

Specifically, for molecular hydrogen (and its heavier isotopes) the lowest resonant state is the $^2\Sigma_u^+$ state of H_2^-. This is a shape resonance, with the X $^1\Sigma_g^1$ state of H_2 as its parent, for internuclear separations less than 3 a.u. The next higher resonant state is the $^2\Sigma_g^+$ state of H_2^-. In

the present calculations we have used the local version of the resonance model and have considered only the $^2\Sigma_u^+$ resonant state of H_2^-.

The relative masses of the six isotopes of molecular hydrogen range from 1 to 3 (in units of the mass of H_2). We have calculated cross sections for the dissociative electron attachment to all six isotopes of H_2. These cross sections are also fitted to useful analytical forms. These attachment cross sections show quite significant isotope effect. We have also calculated a few cross sections for the pure dissociation of three isotopes, namely, H_2, HD and D_2, by electron impact. These dissociation cross sections do not exhibit any significant isotope dependence.

Figure 2 shows the cross sections for dissociative electron attachment to H_2 which has its initial vibrational level as v = 0 or v = 1 or v = 2. Note that the attachment cross section is dramatically enhanced if the attaching molecule H_2 is vibrationally excited. This strong enhancement of the attachment cross section (and, therefore, the attachment rate) on increasing the internal vibrational energy of the molecule is attributed to an increase in the range of internuclear separations over which the electron capture can occur. This increase occurs because of the larger amplitude of vibration for a vibrationally excited molecule. Also note that the cross section shows its peak value at the threshold and it reduces rapidly as the incident electron energy is increased above the threshold. Table 1 provides the threshold energy and the peak value of the cross sections for dissociative electron attachment to vibrationally excited H_2. v is the initial vibrational quantum number of the vibrationally excited molecule.

Figures 3 through 7 show the cross sections for dissociative electron attachment to the heavier isotopes HD, HT, D_2, DT and T_2 which have their initial vibrational levels ranging from v = 0 to v = 3. Once again, note that the attachment cross sections are dramatically enhanced if the attaching molecule is initially vibrationally excited. Also note that, once again, the cross sections show their peak value at the threshold and they reduce rapidly as the incident electron energy is increased above the threshold. However, the magnitude of the attachment cross sections for heavier isotopes is much smaller than the magnitude of the corresponding cross sections for H_2; in fact, the attachment cross section systematically decreases as the isotope mass

increases. It can be qualitatively understood by referring to the resonance model (see Figure 1). The time taken for the separation of the nuclei to increase from the capture radius R_c to the stabilization radius R_s is inversely proportional to $M^{1/2}$ (M is the reduced mass of the nuclei). Thus, nuclei of D_2, taking longer than the nuclei of H_2 to separate out to R_s, experience a stronger competition from electron autodetachment which, in turn, reduces the probability of dissociative attachment. In Tables 2 through 6 are shown the threshold energy and the peak value of the cross sections for dissociative electron attachment to vibrationally excited isotopes HD, HT, D_2, DT and T_2. v is the initial vibrational quantum number of the vibrationally excited molecule.

Since for all six isotopes of H_2 the attachment cross sections show a peak at the threshold and a rapid reduction in magnitude as the electron energy is increased above the threshold, it is quite suggestive to fit the attachment cross sections just above the threshold by an expression of the form:

$$\sigma_{DA}(E) = \sigma_{peak} \exp [- (E - E_{th})/E_o]$$

In order to see the validity and merit of this simple fit we show in Figures 8 through 13 the ratio σ/σ_{peak} for H_2 and its five heavier isotopes as a function of the electron energy above the threshold. Since the attachment cross sections show their peak value at the threshold, the ratio σ/σ_{peak} has the value 1 at threshold and it rapidly decreases as the electron energy is increased above the threshold for attachment. A least squares fit (labeled "Best fit") of all the data to an expression of the form

$$\sigma_{DA}(E) = \sigma_{peak} \exp [- (E - E_{th})/E_o]$$

yields the value of the fitting parameter E_o. This parameter E_o has the value 0.45, 0.39, 0.36, 0.32, 0.30 and 0.28 for the six isotopes H_2, HD, HT, D_2, DT and T_2, respectively.

Assuming a Maxwellian distribution for electron energies, the rate of electron attachment can be written in the form of an analytical expression of the form

$$k(\langle E\rangle) = \left(\frac{27}{\pi}\frac{\langle E\rangle}{m}\right)^{1/2} \sigma_{peak} \exp\left(-\frac{3\,E_{th}}{2\,\langle E\rangle}\right)\left[\left(\frac{3}{2}+\frac{\langle E\rangle}{E_o}\right)^{-2} + \frac{E_{th}}{\langle E\rangle}\left(\frac{3}{2}+\frac{\langle E\rangle}{E_o}\right)^{-1}\right]$$

where $\langle E\rangle = 3\,kT/2$ and T is the electron temperature. This analytical expression can be conveniently used to obtain the attachment rates since σ_{peak}, E_{th}, and E_o are provided, in the present work, for all six isotopes of H_2.

Finally, Figures 14 through 16 show resonant contributions to the cross sections for pure dissociation of H_2, HD and D_2 by electron impact for various initial vibrational levels of the molecule. Note that in this case, unlike the dissociative electron attachment case, the cross sections neither show any noticeable isotope effect nor are enhanced significantly upon initial vibrational excitation of the molecule.

List of publications by J. M. Wadehra during the period of the CRP.

1. "K-shell ionization of atoms by electron impact", S. P. Khare and J. M. Wadehra, Phys. Letts. A198, 212 (1995).

2. "Scaling relations for L-shell ionization cross sections of atoms by electron and photon impacts", S. P. Khare, P. Sinha and J. M. Wadehra, Ind. J. Phys. B69, 219 (1995).

3. "Electron Attachment to Molecules at Low Electron Energies", A. Chutjian, A. Garscadden and J. M. Wadehra, Physics Reports 264, 393-470 (1996).

4. "K-, L- and M-shell ionization of atoms by electron and positron impact", S. P. Khare and J. M. Wadehra, Can. J. Phys. 74, 376 (1996).

5. "A quasifree model for the absorption effects in positron scattering by atoms", D. D. Reid and J. M. Wadehra, J. Phys. (Letters) B29, L127 (1996).

6. "Intermediate to high energy positrons scattered by alkali atoms", D. D. Reid and J. M. Wadehra, Phys. Rev. A57, 2583 (1998).

Brief Report on the Activities within the Project: "Cross Sections and Kinetics in Divertor Plasmas" (RA No. 8619/CF)

CSI: M. Capitelli
Dept. of Chemistry, Research Centre of Plasma Chemistry, University of Bari, Italy

In the period interesting the present CRP(95-99) the group of Bari worked on different topics dealing with H_2 and D_2 plasmas which can be summarized as follows

Atomic and Molecular Physics

1) State to state electron molecule(H_2, D_2, T_2) excitation cross sections

In this section we have performed calculations by using the semiclassical impact parameter approximation on electron-H2 inelastic collisions. Complete sets of excitation and dissociation cross sections involving the whole vibrational ladder of ground state and electronically excited molecules have been obtained.

Cross sections for the different isotopes have been obtained either by using the impact parameter method or by using appropriate scaling laws. A complete report on these results is in preparation.

2) State to state vibrational deactivation cross sections of H_2, D_2 on copper surface; state to state recombination cross sections of atomic hydrogen on copper and graphite

Point 2 has been developped by a collaboration between Cacciatore(Bari) and Billing(Copenhagen). These authors have developped a semiclassical approach for studying the molecular dynamics of vibrationally excited H_2 and D_2 molecules impinging on copper surfaces as well as the the recombination of atomic hydrogen on the same surfaces covered by physiabsorbed hydrogen. In the last case a strong nen-equilibrium nascent vibrational distribution of H_2 has been observed.

3) State to state excitation and dissociation cross sections of H_2, D_2 colliding with atomic H and D

We have recently calculated a complete set of excitation and dissociation cross sections of vibrorotationally excited H_2 molecules impinging with atomic hydrogen. We have used the classical trajectory method on the best available potential energy surface. The cross sections have been then used in a kinetic scheme obtaining a global dissociation constant as a function of gas temperature. The results are in very good agreeement with the corresponding experimental ones thus confirming the accuracy of the whole set of cross sections.

Kinetics

1) Development of a collisional-radiative model for $H_2(v)$, H(n) species

In collaboration with K.Hassouni and A.Gicque(Universite' de Paris Nord) a new collisional radiative model for H2 plasmas has been developped. This model includes a collisional radiative model for vibrationally and electronically excited molecular species as well as for electronically excited atomic hydrogen. These kinetics are coupled to an appropriate Boltzmann equation describing the electron energy distribution function(eedf) and to the ion kinetics for both positive and negative ions. Finally a transport equation is used for describing the diffusion of species on solid substrate. The model has

been in particular applied to microwave discharges but can be easily extended to edge plasma conditions.

2) Role of attachment from Rydberg states

The above collisional radiative model has been applied to understand the role of Rydberg states in affecting the production of negative ions. It has been shown that both for microwave discharges and for multicusp magnetic ones dissociative attachment from Rydberg states is a channel competitive with the corresponding production by attachment from vibrationally excited states thus reinforcing the importance of Rydberg states in the kinetics of negative ions.

3) Decay of eedf in electronically and vibrationally excited H_2 post discharges

The collisional radiative model has been also applied to follow the decay of electron energy distribution function under post discharges conditions. The results shows a well structured eedf as a result of superelastic collisions from both vibrationally and electronically excited states. In particular the metastable 2s state of atomic hydrogen plays an important role during the whole relaxation.

4) PIC-MCC for RF H_2 discharges

A particle in cell with Monte-Carlo collisions has been developped to follow the hydrogen kinetics in RF plasmas. The studied conditions emphatize also the possibility of usiong such discharges for the formation of negative ions.

Transport

1) Collision integrals of excited H(n) states

Elastic and transport cross sections of H(n)-H(n) collisions with n up to 5 have been calculated by using a quantum mechanical dynamic approach with potential energy curves derived from a full CI(configuration interaction) approach. The results which show a strong increase of cross sections with the principal quantum number n can be used to evaluate the the role of electronically excited atoms in affecting the transport properties of non-equilibrium plasmas.

2) Transport properties of one and two temperature H_2 plasmas

The last topics includes a new evaluation of transport coefficients(total thermal conductivity, viscosity and electrical conductivity) for themal one or two temperature plasmas.

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Brief Report on Activities on the Project:
"Charge exchange and associative ionization in low-energy collisions of H and H^-"

Prof. F. Brouillard (RA No. 8605/CF)

1. Absolute cross sections have been measured for the following **rearrangement processes involving the negative hydrogen ion H^- and a positive ion.**

a. electron transfer

$$H^- + He^+ \rightarrow H + He$$
$$H^- + Ne^{3+} \rightarrow H + Ne^{2+}$$
$$H^- + Ar^{3+} \rightarrow H + Ar^{2+}$$

b. associative ionisation

$$H^- + He^+ \rightarrow HeH^+ + e$$
$$D^- + He^+ \rightarrow HeD^+ + e$$
$$H^- + H_2^+ \rightarrow H_3^+ + e$$
$$D^- + H_2^+ \rightarrow H_2D^+ + e$$
$$H^- + D_2^+ \rightarrow HD_2^+ + e$$
$$D^- + D_2^+ \rightarrow D_3^+ + e$$
$$D^- + C^+ \rightarrow CD^+ + e$$

All the cross sections were measured using a new merged beam apparatus, capable of an accurate determination of the beam geometrical overlap (so-called form factor) .
Many of the measurements have also been carried out in the so-called "animation" mode, where the two beams are moved against each other, perpendicularly to their common axis, in a regular, two-dimensional scanning movement.
In this mode, the reaction rate becomes independent of the interaction geometry so that the cross section measurements are not affected by possible fluctuations of the form factor.
As a result, the accuracy of the results is claimed to be better than 5%.

For electron transfer, the measurements have covered a very wide range of collision energies, from 1 eV to 3 000 eV.
They also included measurements of the exothermicity of the reaction, by an analysis of the time of flight of the products. This permitted an identification of the quantum states of the products.
A close coupling calculation of the electron transfer from H^- to a positive ion was carried out, in which the system is treated as a three electron one.

For associative ionisation, the energy range covered was 0.01 eV- 10 eV.
Cross sections are found to be large, especially for the formation of the CD^+ ion.
Their energy (E) dependence obeys in all cases an E^{-1} law at low energy, up to 1 eV.

2. Experimental work has also been continued on
associative ionisation in the collision of two hydrogen atoms.

The H-H collisional system is an important one not only because of its direct relevance to thermonuclear fusion and astrophysics but also because it is especially appropriate to test the theoretical models proposed for molecular dynamics.
The following reactions had been investigated previously

$$H(1s) + H(2s) \rightarrow H_2^+ + e$$
$$D(1s) + D(2s) \rightarrow D_2^+ + e$$
$$D(1s) + D(2s) \rightarrow D_2^+ + e$$

During the present RCP, the experimental set-up has been coupled to a dye laser and equipped with optical instrumentation to produce, from the beam of metastable atoms, intense beams of atoms in higher excited states .

Measurements have been successfully carried out of the cross section of the reaction

$$D(1s) + D(3s) \rightarrow D_2^+ + e$$

over the energy range 0.005 eV- 4 eV.

Measurements are now in progress for the reactions

$$H(1s) + H(3s) \rightarrow H_2^+ + e$$
$$H(1s) + H(nl) \rightarrow H_2^+ + e$$
$$D(1s) + D(nl) \rightarrow H_2^+ + e$$

3. Intensive experimental work has also been carried out on **electron impact ionisation of multiply charged ions and ionisation or dissociation of molecular ions.**

Absolute cross sections have been measured, using animated crossed beams, of the following reactions

a) simple ad double ionisation of multiply charged ions of Ne

$Ne^{q+} + e \rightarrow Ne^{(q+1)+} + 2e$	$q = 4$ to 8	from threshold to 5 000 eV
$\rightarrow Ne^{(q+2)+} + 3e$	$q = 5$ and 6	idem

b) simple, double and triple ionisation of multiply charged ions of Ni

$Ni^{q+} + e \rightarrow Ni^{(q+1)+} + 2e$	$q = 10$ to 15	from threshold to 4 000 eV
$\rightarrow Ni^{(q+2)+} + 3e$	$q = 10$ to 15	from threshold to 5 000 eV
$\rightarrow Ni^{(q+3)+} + 4e$	$q = 12$	from threshold to 3 000 eV

c) ionisation, dissociation and dissociative ionisation of molecular ions

$0_2^+ + e \rightarrow O^{++} + O + 2e$		from threshold to 2 500 eV
$\rightarrow O^+ + O + e$		
$N_2^+ + e \rightarrow N^{++} + N + 2e$		idem
$\rightarrow N^+ + N + e$		
$C0^+ + e \rightarrow CO^{++} + 2e$	idem	
$\rightarrow C^{++} + O + 2e$		idem
$\rightarrow C + O^{++} + 2e$		idem
$C0_2^+ + e \rightarrow CO_2^{++} + 2e$		idem
$\rightarrow C^+ + O_2 + e$		idem
$H_20^+ + e \rightarrow H^+ + OH + e$		idem
$\rightarrow O^{++} + H_2 + e$		idem
$H_30^+ + e \rightarrow H_3O^{++} + 2e$		idem
$\rightarrow H^+ + H_2O + e$		idem
$\rightarrow H_2^+ + OH + e$		idem

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A. Siari, D.S. Belic, P. Defrance and S. Rachafi
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17. **Electron impact double ionisation of C^- and O^- ions.**
C. Bélenger, D. Belic, D.J. Yu and P. Defrance
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18 **Electron impact ionisation of Nickel multiply charged ions.**
S. Cherkani-Hassani, P. Defrance and E. M. Oualim
Physica Scripta (1999) in press

Recent Activities in CRP on "Atomic and Molecular Data for H, He and Their Ions Relevant to Divertor Plasma Analysis"

H.Tawara (NIFS, Toki, Japan)

The members of this CRP group consist of

A.Ichihara (JAERI)
K.Onda (Science University of Tokyo)
T.Shirai (JAERI)
K.Sakimoto (ISAS)
H.Takagi (Kitasato Univ.)
H.Tawara (NIFS).

The main aims of this group are to collect, calculate and evaluate the collision data involving H, H_2, He and their ions at low energy region which are requisite in understanding and modeling the divertor plasmas. In the previous two CRP meetings we had described the present situations for these collision data. In the 1997-98 period we are continuing new calculations and also compilation of such data.

I) The main activities can be summarized as follows :

1) Quantum mechanical calculations of collinear He + $H_2^+(v_i)$ collisions at low energies :

The present theory [1] had been previously used and tested to calculate the collision probabilities and cross sections for different collision systems such as H + $H_2(v_i)$, $H_2(v_i)$ + $H_2(v_i')$ and He + $H_2(v_i)$ as a function of the initial vibrational state v_i of molecule.

The following three processes are considered in the present calculations :

$$He + H_2^+(v_i) \rightarrow He + H_2^+(v_f) \quad (1.1)$$

$$\rightarrow HeH^+(v_f) + H \quad (1.2)$$

$$\rightarrow He + H^+ + H \quad (1.3)$$

over the collision energy range of 4 - 10 eV and over all the vibrational states up to $v_i = 17$.

The important results in the present calculations of probabilities have been concluded as follows :

a) Strong undulations are clearly observed among the probabilities for these three processes.
b) Process (1.2) is dominant at low v_i in all the collision range.
c) Process (1.3) is dominant for large v_i.
d) The change of the vibrational states in process (1.2) before and after collisions is small, and mostly $\Delta(v_i - v_f) = 1$.

Also preliminary calculations have been performed to see the effect of different isotope combinations on collinear collisions in $^4He + HT^+$ and $^4He + TH^+$ systems for $v_i = 1 - 8$.

e) For small v_i, the vibrational transitions are dominant in both collision combinations at all the collision energies, though there is clear indication that the dissociation process increases in $^4He + TH^+$ collisions at higher energies.
f) For large v_i, the dissociation in $^4He + TH^+$ collisions becomes dominant over other processes, particularly at high energies.

These features can be qualitatively understandable due to the mass difference between two colliding partners on a collinear line.

2) Semiclassical calculations of dependence on the initial rotational and vibrational states (j_i and v_i) in low energy $H^+ + D_2(j_i, v_i)$ collisions :

Using the trajectory surface hopping method combined with *ab initio* three-dimensional potential energy surfaces which has been described in detail previously [2.1], the cross sections for the following processes

$H^+ + D_2(v_i) \rightarrow H + D_2^+(v_f)$ (2.1)

$\rightarrow HD^+(v_f) + D$ (2.2)

$\rightarrow D^+ + HD(v_f)$ (2.3)

$\rightarrow H + D^+ + D$ (2.4)

have been calculated over the parameter ranges of E_{cm}= 2.5 - 8.0 eV, v_i = 0 - 3 and j_i =1, 5 and 10.

The present calculations indicate the following important aspects :

a) Process (2.1) is significantly enhanced as v_i increases but less with j_i.

b) Processes (2.2) - (2.4) do depend only weakly on v_i but are practically independent of j_i.

II) The details of these results in the 1997-98 activities described above can be found in the following publications :

1) K.Onda and K.Sakimoto : J. Chem. Phys. (submitted 1998)
Quantum mechanical study on energy dependence of probabilities on non-reactive vibrational transitions, atom exchange reaction and dissociation in a collinear He + $H_2^+(v_i)$ collision

2) A.Ichihara : JAERI-DATA/Code 98-031 (1998)
Potential energies for the lowest $^1A'$ electronic states of H_3^+

3) A.Ichihara : JAERI Research 98-056 (1998)
Cross sections for ion production in reactions of H^+ with D_2 : effects of vibrational and rotational excited states

4) T.Tabata, T.Shirai, H.Tawara and R.Ito : J. Phys. Chem. Ref. Data (submitted, 1999)
Cross sections for collisions of electrons with edge plasma impurities

5) T.Tabata and T.Shirai : JAERI Memo (1999)
Analytic cross sections for collisions of H^+, H_2^+, H_3^+, H, H_2 and H^- with hydrogen molecules

III) References

[1.1] K.Sakimoto and K.Onda : J. Chem. Phys. **100** (1994) 1171
[2.1] A.Ichihara, T.Shirai and K.Yokoyama : J. Chem. Phys. **105** (1996) 1857

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Macedonia

Low-energy Collision Processes of Ions with Atoms and Solid Surfaces

(Progress Report for 1995/11/15-1998/11/14)

Principal Investigator

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Using the adiabatic superpromotion model of low-energy atomic collisions, a simple scaling relationship was derived for the ionization cross section of hydrogen atoms colliding with multiply charged ions. Detailed ionization-cross-section calculations for $H(1s)+He^{+}$, C^{6+}, and O^{8+} have been performed and used to determine three numerical constants in the cross-section-scaling relationship. The scaled cross section represents well the available data for fully stripped ions with charge $Z>1$ in the energy region below the cross-section maximum.

A classical description of state selective excitation processes in atom-charged particle collisions was provided for arbitrary values of collision energy. Closed-form expressions for the cross sections of $nl\rightarrow n'$, $nl\rightarrow l'$ and $nl\rightarrow n'l'$ transitions are obtained in the high energy limit. The scaling properties of $\sigma(nl\rightarrow n'l')$ cross sections were analyzed.

Using the advanced adiabatic method the cross sections for excitation, ionization and electron capture of H(1s) and H(2s) colliding with Li^{3+} have been calculated in the energy ranges 0.1-20 keV/u and 0.1-7 keV/u, respectively. All radial and rotational couplings among the adiabatic states with united atom principal quantum number $N<10$ have been included in the calculations, as well as the electron promotion to the continuum via the S- and Q- superseries of hidden crossings. The obtained results were compared, when possible, with the results of other cross-section calculations or measurements

The method of hidden adiabatic energy crossings in the complex plane of internuclear distance was employed to calculate the total, shell- and subshell-selective electron capture cross sections in $Be^{4+}+H(1s)$ collisions in the energy range 0.1-10 keV/u. The calculations extend considerably the existing cross section data for these processes in the low energy region

The structure of the hidden crossings of the adiabatic potential curves in the two Coulomb centers problem with charges Z_1 and Z_2 has been studied when $Z_1<<Z_2$. In this case new type of hidden crossings between the states (n,l,m) –(n,l+1,m) was revealed.. The inelastic transitions via such hidden crossings in $O^{7+}+H^{+}$ collisions have been calculated.

The impact parameter dependence of the transition probability for $He^{2+}+H(1s)$ $\rightarrow He^{+}(n=2)+H^{+}$ and $He^{+}(1s)+H^{+}\rightarrow He^{2+}+H(1s)$ electron transfer reactions at collision energies of 3 and 2 keV/u ,respectively, was calculated within the advanced adiabatic method with inclusion of the dynamical phases and the topological phase associated with the corresponding hidden crossing branch point of the adiabatic electronic energy in the complex plane of internuclear distance. The results of the calculations were compared with those of multi-channel close-coupling calculations based on a molecular orbital expansion. The effect of the topological phase is to alternate the oscillatory structure of the transition probability.

The hidden crossings of rotational energy levels of H_2O molecule embedded in an external electric field were studied. It was found conditions when the relevant non-adiabatic transitions become significant

The problem of determination of momentum distributions of ejected electrons in slow atomic collisions was studied within the impact parameter method by using a dynamic adiabatic basis which takes into account the correct boundary conditions. An expression was obtained which relates the momentum distribution of ejected electrons with a

coherent sum of the delocalized dynamic adiabatic eigenstates (elementary wavepackets). The form of the momentum distribution exactly coincides with the form of the total wavepacket in configuration space. General formulas were applied to a model problem of electron detachment in the process $A^-+A \rightarrow A+A+e$ in which the electron-atom interaction are described by the zero-range potentials. In the example considered , the momentum distribution of ejected electrons, in the center of mass frame , exhibits a maximum located in scattering plane on the circle of the radius $k=(v/\rho)^{1/2}$, where v is the relative velocity and ρ is impact parameter

List of resulting publications

1. Grozdanov T.P. and Solov'ev E.A. HIDDEN CROSSINGS AND THE SEPARATION CONSTANT OF A HYDROGENLIKE ATOM IN SPHEROIDAL COORDINATES. Phys.Rev. A51, p.2630 (1995)

2. Solov'ev E.A. THE LOW-ENERGY ATOMIC COLLISION THEORY. Book of Invited Lectures XIX Int.Conf.Phys.Elec.At.Col., Ed. by J.B.A.Mitchell, J.W. McConkey, C.E.Brion, p.45, Whistler, 1995

3. Savichev V.I. and Solov'ev. E.A. NEW TYPE OF HIDDEN CROSSINGS IN ATOMIC COLLISIONS WITH PARTICIPATION OF HIGHLY CHARGE IONS. Phys.Lett.A. 205, 184 (1995)

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5. Janev R.K., Solov'ev E.A. and Wang Yi. ELECTRON CAPTURE, EXCITATION AND IONIZATION IN SLOW COLLISIONS OF LI^{3+} IONS WITH GROUND-STATE AND METASTABLE HYDROGEN ATOMS. J.Phys.B. 29, 2497 (1996)

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8. Janev R., Solov'ev E.A., TOPOLOGICAL PHASE AND INTERFACE EFFECTS IN SLOW He^{2+}+H AND He^{+}+H^{+} CHARGE EXCHANGE COLLISIONS J.Phys.B: At. Mol. Opt. Phys. 30 L353-L360 (1997)

9. Solov'ev E.A., HIDDEN-CROSSINGS AND NON-ADIABATIC TRANSITIONS BETWEEN ROTATIONAL STATES OF H_2O IN SLOW VARYING EXTERNAL FIELD, Phys. Lett. A 249, p.74, (1998)

10. Macek J., Ovchinnikov S.U., Solov'ev E.A., ELECTRON ENERGY AND ANGULAR DISTRIBUTION IN A SOLVABLE MODEL OF ION-ATOM COLLISIONS, Phys. Rev. A (accepted)

11. Grozdanov T.P., Solov'ev E.A., ADVANCED ADIABATIC THEORY FOR MOMENTUM DISTRIBUTIONS OF EJECTED ELECTRONS IN SLOW ATOMIC COLLISIONS, Eur. Phys. J. (accepted)

12. Janev R.K, Solov'ev E.A., Stephens J.A., STATE-SELECTIVE AND TOTAL ELECTRON CAPTURE, EXITATION AND IONIZATION CROSS SECTIONS IN SLOW COLLISIONS OF H(2s) AND $He^+(2s)$ WITH H^+, He^{2+}, Li^{3+}, Be^{4+} and B^{5+}, Report of International Nuclear Data Committee, INDC(NDS)-393 (1999)

E.A.Solov'ev

Report on the the research project n°10317 of the CRP 'Atomic and plasma walls interaction data for fusion reactor divertor modelling'. CSI: C.Harel.

INTRODUCTION

Currently, chemical species with nuclear charges $Z < 8$ are found in the plasmas of operating tokamak devices; furthermore, ion temperature depends on their location: in the plasma core, ion temperatures up to a few keV/amu are observed whereas close to the walls they are much lower (down to energies of a few eV/amu).

We have performed molecular calculations for total and state selective electron capture and ionisation cross sections in collisions between multicharged ions with charges $Z \leq 8$ and atomic hydrogen- H(1s) and H(2s)- for the nuclear projectile energy range 62.5 eV/amu < E < 25 keV/amu. Classical calculations have been carried out for the same systems for energies up to 2.5 MeV/amu for ionisation and 625 keV/amu for charge transfer.

In the same impact energy range, we have also calculated total and state selective charge transfer and ionisation cross sections in collisions of the same projectiles with H_2 molecules .

THEORY

We have used the molecular approach of atomic collisions which is known to provide reliable electron capture cross sections in the energy range considered here. A full quantal treatment is used for low impact energies (E<0.1 keV/amu); at higher impact energies, a semiclassical treatment with rectilinear trajectories for nuclear motion has been found accurate. At very high impact energies (E>25keV/amu) we employ an eikonal CTMC formalism with a hydrogenic initial distribution. Finally, either a common reaction coordinate formalism (quantal treatment) or a common translation factor (semiclassical treatment) are used to account for the electron momentum transfer problem.

Energies and couplings of the quasi-molecules are calculated using an OEDM basis set. In the case of non bare nuclei (He-like ions) the effect of the $1s^2$ electronic core on the active electron is taken into account using a model potential approach. In the later case, a correction to the H_2^+-like- OEDM- molecular basis set is made by an interaction method (compact gaussians orbitals are added to the molecular expansion) in order to improve the molecular data that is required at low impact energies (v<0.2 a.u.).

In ion-molecule collisions, we have used the sudden approximation to treat the vibro-rotational motion of the molecule. At low energies (E<1keV/amu), we have employed an ab initio method to calculate potential energy surfaces and dynamical couplings. At intermediate energies (250eV/amu<E<25keV/amu), a model potential has been used to describe the molecular target. At low and intermediate impact energies we have calculated state-to state vibrational electron capture and transfer dissociation cross sections. At high energies (E>25keV/amu), the CTMC-model potential formalism has been applied .

RESULTS

1 . Ion-atom molecular calculations.

H^+-H(ls) collisions:
The molecular basis includes all states correlating to excitation and capture channels up to n=6, (*112 states*). Cross sections are tabulated for n=1-4.

He^{2+}-H(ls) collisions:
The molecular basis includes all states correlating to excitation and capture channels up to n=3 and 6 respectively (*66 states*).
Cross sections are tabulated for n=1-4

Li^{3+}-H(1s) collisions:
The molecular basis includes all states correlating to excitation and capture channels up to n=2 and 7 respectively (*88 states*). Cross sections are tabulated for n=2-5.

Be^{4+} -H (1s), H(2s) collisions:
The molecular basis includes all states correlating to excitation and capture channels up to n=2 and 7 respectively (*88 states*). Cross sections are tabulated for n=2-5. A comparison between quantal and semiclassical calculations has shown that for v<0.03 a.u. (E<22.5 eV/amu) a full quantal treatment was necessary: *the use of a common coulombic trajectory for the nuclear motion doesn't improve the semiclassical results.*

B^{5+}-H (ls) collisions:
The molecular basis includes all states correlating to excitation and capture channels up to n=2 and 7 respectively (*88 states*). Cross sections are tabulated for n=3-6.

C^{6+}-H(1s) collisions:
The molecular basis includes all states correlating to capture channels up to n=8 (121 states. Cross sections are tabulated for n=3-6.

N^{7+},O^{8+}-H(ls) collisions:
The molecular basis includes all states correlating to capture channels from n=4 to n=7 and the states of symmetry m=0, 1 and 2 correlating to n=8 and 9 capture channels (*129 states*).
Cross sections are tabulated for n=4-7.

C^{4+} -H (1s) collisions:
Total and partial cross sections for capture onto n=3,4 have been calculated for impact energies from 10 eV to 25 keV.

2. Ion-atom CTMC calculations.

Total electron capture and ionisation cross sections for bare ions (**H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}** and **O^{8+})-H(1s)** collisions.

3. Ion-molecule semiclassical calculations.

H^+-H_2 collisions.

Two-state ab initio calculations were carried out including the entrance channel and the molecular state dissociating into H (1s)+H_2^+ ($1\sigma_g$). In the model potential treatment states correlating to H(n=2,3) + H_2^+ , together with the first three excited states of H_2 were added to the basis set. Calculations were carried out at the Franck Condon level.

Be^{4+} -H_2 collisions

Ab initio calculations included the molecular states dissociating into Be^{4+} -H_2 and Be^{3+}(n=3) + H_2^+. Partial single electron captures vibrational cross sections were calculated using the sudden approximation. A block-diagonalization technique was used to calculate single capture states that lie in the ionisation continuum. In the model potential treatment, states correlating to Be^{3+}(n=3, 4) + H_2^+ were included in the basis set. Calculations were carried out at Franck Condon level.

C^{4+} -H_2 collisions

Ab initio calculations included the molecular states dissociating into C^{4+} -H_2 and C^{3+}(n=3) + H_2^+. Partial vibrational single electron capture cross sections were calculated using the sudden approximation. . A block-diagonalization technique was used to calculate single capture states that lie in the ionisation continuum. In the model potential treatment, states correlating to C^{3+}(n=2, 3 and 4) + H_2^+ where included in the basis set. Calculations were carried out at Franck-Condon level.

C^{3+} -H_2 collisions

Ab initio calculations included 7 molecular states dissociating into C^{3+} -H_2, C^{2+}+ H_2^+ and C^++H^++H^+. Single and double electron capture cross sections were calculated at Franck-Condon level.

C^{2+} -H_2 collisions

Ab initio calculations were carried out for single electron capture processes from the ground state $C^{2+}(1s^2 2s^2, {}^1S)$ and from the metastable state $C^{2+}(1s^2 2s\ 2p, {}^3P)$. From the calculated charge transfer cross sections we have obtained the proportion of metastable ions in the incident experimental beam.

N^{5+}- H_2 collisions

Ab initio and model potential calculations have been carried out at the Franck-Condon level. Partial cross sections to $N^{4+}(1s^2$ n=3, 4) + H_2^+ have been obtained. Ab initio calculations have pointed out the importance of double charge transfer into the autoionizing levels $N^{3+}(1s^2 3l3l')$.

Li^+ - H_2 collisions

Five states ab initio calculations have been carried out for single electron capture and target excitation. The strong anisotropy of the cross sections has been pointed out.

4. Ion-molecule CTMC calculations

Total electron capture and ionization cross sections for bare ions (H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+})-H_2 collisions.

CONCLUSION

Intensive calculations involving non bare Helium-like nuclei are now in progress according with our plans for the CRP. In parallel, during the last few years we have extended our field of investigation in two directions: i) ion-atom collisions at intermediate impact energies and treatment of the ionisation process in the molecular close coupling approach and ii) neutralisation of slow highly charged ions at metallic surfaces. Both allow future studies of interest for other aspects of the controlled fusion as for instance heating by neutral injection and ions/walls interactions.

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Research Project AUS-10370/CF „Electron impact ionization and surface induced reactions of edge plasma constituents"

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1. General introduction:

Recent studies in the field of thermonuclear fusion based on magnetic confinement of high temperature plasma have demonstrated that the conditions at the plasma periphery („plasma edge") play an important role for achieving, sustaining and controlling the thermonuclear fusion. In order to understand and elucidate the role of the radiative and collisional processes in this plasma region, it is essential to have available detailed and quantitative knowledge on the corresponding elementary reactions proceeding in the volume and at the wall. Moreover, as high current H^- ion sources are of potential interest in fusion research also negative ion formation and reactions are of special interest.

Today's situation in terms of accurate data on these processes is far from satisfying (see R.K.Janev, Plenum, 1995 and W.O.Hofer,J.Roth, Academic, 1996). The present project includes three areas of study in order to provide *quantitative information* on collision processes involving various plasma edge constituents (the various particles have been specified in several reports written by fusion experts, see above):
(i) Experimental studies about electron ionization of neutrals and ions and electron attachment to molecules,
(ii) Theoretical studies about electron ionization of neutrals and ions and
(iii) Reactive interaction of molecular ions with surfaces.
It was possible to achieve progress in all three of these areas since the beginning of this co-ordinated research programme and in particular in the past months. In section 2 a brief outline of the results obtained will be given for each sub-field. This will be followed by an appendix containing a list of publications [1] - [121] based on work carried out and related to the CRP (1995 - present).

2. Results

2.1.Experimental studies about electron ionization of neutrals and ions

2.1.1. Determination of partial and total cross sections, kinetic energy releases and ionization energies:

The experimental crossed-beams sector-field mass-spectrometer (CSM) set-up and the procedure used in our laboratory for the accurate measurement of partial ionization cross sections of atoms and of molecules consists of a modified Nier-type electron impact ion source, a molecular beam source (either a Knudsen-type oven or a nozzle expansion source) and a high resolution double focusing two-sector field mass spectrometer. The performance and operating conditions of this apparatus have been continuously improved over the past 15 years. Today it is possible to measure (absolute) total ionization cross sections and partial ionization cross section functions for atomic and molecular parent ions as well as partial ionization cross section functions for fragment ions formed with excess kinetic energy with high accuracy up to electron energies of 1000 eV. This was tested in detail with CF_4 and used recently for the study of the two fusion plasma relevant substances C_2H_6 and C_3H_8 (in addition first studies on carbon aggregates have been started).

As shown in these studies it is (i) necessary (in order to account quantitatively for discrimination effects in the case of fragment ions produced with excess kinetic energy in the ion source) and it is (ii) also possible to measure the kinetic energy release distributions (KERD) of the fragment ions formed by electron impact ionization in the ion source using a method developed over the years in our laboratory (this ion beam deflection method is based on the fact that the extracted ion beam shape contains information on the original ion kinetic distribution of the ions produced by electron ionization of the neutral targets). Detailed studies about KERD's and the average total kinetic energy release (KER) deduced from these distributions have been performed recently for C_3H_8 and are presently in addition pursued with a newly developed (mass analyzed retarding potential, MARP) method using the tandem mass-spectrometer (TM) apparatus described in section 2.3 (first results have been obtained for CH_4 and C_3H_8 [10]). These measurements have been complemented by MIKE (mass analyzed ion kinetic energy) studies about the metastable (spontaneous) decay of mass selected molecular ions, in particular various propane ions.

Moreover, using monochromatized electrons (from a hemispherical electron monochromator HEM) in a newly constructed high resolution crossed-beams/quadrupole mass spectrometer (CQM) apparatus we were able to (i) measure in great detail the ionization threshold region and thus to (ii) deduce ionization energies; first examples of this include ionization energies for various rare gases, molecules and aggregates.

In concluding this section, the joint use of the three apparatus developed in our laboratory (CSM,CQM,TM) allows us now to provide a complete quantitative account of the kinetics (cross sections) and the energetics (ionization energy, kinetic energy release) of the electron impact ionization of molecular targets. Measurements have been carried out for the prototypical linear hydrocarbon molecule C_3H_8 and started for the CH_4 molecule.

Moreover, as high current H^- ion sources are of potential interest in future fusion reactors we have also started high resolution electron attachment studies with the HEM/CQM machine and a recently constructed high resolution trochoidal electron monochromator (TEM) apparatus including investigations for O_2, NO, CO and CO_2.

2.1.2. Electron impact ionization/dissociation of mass selected molecular ions

In order to study electron induced ionization and dissociation of mass selected molecular ions, we have recently modified the two sector field mass spectrometer system (CSM) in such a way as to allow with help of a newly constructed high performance electron gun the study of inelastic interactions between electrons and ions in the ion beam focus of the second field free region (half way between the magnetic and the electrostatic field). Ions passing this second field free region have already been mass selected by the magnetic sector field. Because ions are produced in this set-up by an ordinary electron-impact ionization Nier type ion source the primary ion currents available after mass selection are in the order of about 10 pA. With the present electron gun (with electron currents of about 10 mA) mounted between the two sectors it became possible to investigate electron induced ionization and fragmentation of mass selected ions. In particular we used the MIKE-scan (mass analyzed ion kinetic energy scan) in order to identify and analyze fragment ions in terms of their mass and charge state and their kinetic energy release. The position and height of the respective MIKE peaks allows an unambiguous quantitative identification of the parent and fragment ions produced and from the shape of a MIKE peak it is possible to derive the total kinetic energy release distribution (KERD) of a specific decay reaction. In a further step the average total kinetic energy release (<KER> value) of the decay reaction can be determined by calculating the first momentum of the KERD. After testing this method in detail we have recently measured and studied the ionization of various propane ions as a first prototypical case and also of CO_2. In this latter case we have also been able to determine the partial and (energy) differential cross sections for the ionization and dissociation of the selected parent ion (step-wise-ionization).

In addition, we have added to this two sector field mass spectrometer system a third sector (electrostatic sector field), thus constructing a three sector field machine which will allow us to study in much more detail and generality ionization reactions mentioned in 2.1. This three sector field machine has been built and tested the past months and will soon be ready for the first measurements.

2.2. Theoretical studies about electron ionization of neutrals and ions

Scaling laws and semiempirical methods can be powerful tools to predict electron impact ionization cross sections for neutrals and ions for modeling purposes in particular for those targets where experimental data do not exist and/or rigorous theoretical calculations are inconvenient or impossible. Many practical applications require either a quick estimate of a large number of ionization cross sections or ionization cross section functions in analytical form. Because classical, semi-classical and semi-empirical formulae fail in certain even simple cases, we have suggested in 1987 (called today „DM concept") the use of a semi-classical approach based on a combination of the binary encounter approximation and the Born-Beth approximation.

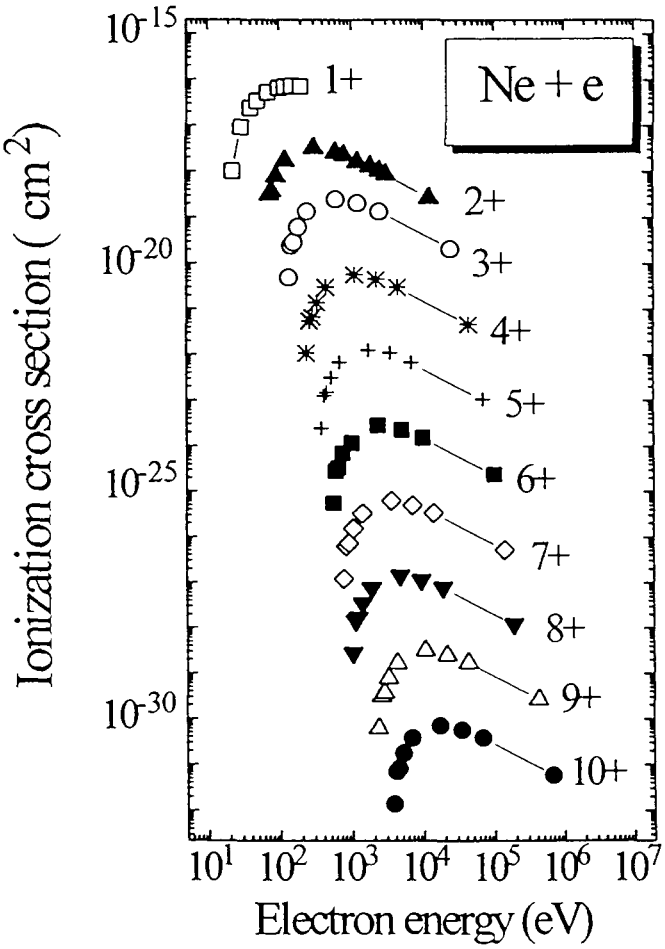

Fig.1 Calculated cross section functions (using the modified DM approach) for the formation of singly and multiply charged Ne^{z+} ions via electron impact ionization of Ne.

Although originally devised for the single ionization of ground state atoms, this DM concept has been successfully extended to the single ionization of excited atoms, free radicals , molecules, clusters and atomic ions. We have now started to apply this DM concept to the case of multiple ionization of atoms (e.g., including up to tenfold ionization of Ne as shown in Fig.1 and 14fold ionization of Si) and a modified additivity rule concept MAR to the single ionization of molecules consisting of several different atomic species. In addition we have applied (and partially improved) this DM formalism treating single ionization of alkali atoms, single ionization of Ag atoms and Ag aggregates and K-shell ionization of atoms.

Moreovers in the framework of a collaboration with Prof.H. Summers and Culham in order to incorporate these multiple ionization processes into the ADAS code we have derived reaction rate coefficients derived from the cross sections given in Fig.1 (see Fig.2).

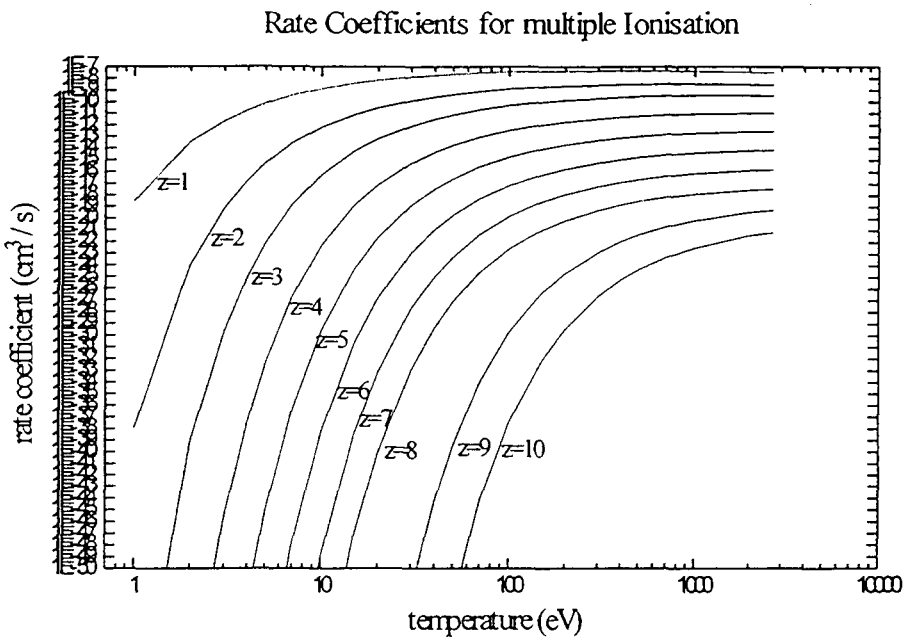

Fig.2 Reaction rate coefficient as a function of electron temperature T derived from the calculated cross sections (see Fig.1) for the formation of singly and multiply charged Ne^{z+} ions via electron impact ionization of Ne.

2.3. Reactive interaction of molecular ions with surfaces („surface erosion")

Recently we have constructed in our laboratory a new tandem mass spectrometer (TM) consisting of an ion source, a two sector field mass spectrometer, a deceleration ion optics, a surface collision chamber and a time of flight mass spectrometer. This apparatus allows us to study the various surface induced reactions such as surface induced dissociation, ion surface reactions and chemical sputtering as a function of collision energy (from threshold up to about 3 keV). Thus we are now able to obtain information about the mechanisms, the kinetics and the energetics of the reactions occurring. After first tests we have so far studied prototypical reactions (using also deuterated species) of acetone monomer and cluster ions, benzene ions, fullerene ions and CF_x^+ ions with a hydrocarbon covered stainless steel and gold surface as a function of the primary collision energy and for various degrees of aggregation of the incoming projectile.

In addition, experimental work on the interaction of hydrocarbon ions with carbon tiles from the Tore Supra from Cadarache (see below and also Fig.3) has been carried out in collaboration with the Euratom/ÖAW Association project P2 of Prof.F.Aumayr.

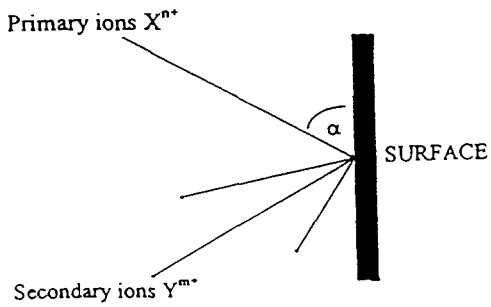

Fig.3 Hydrogen/carbon recycling experiment in collaboration with Tore Supra, Cadarache and AIP, TU Wien. Primary ions X: C^+, C^{2+}, C^{3+}.. , H^+, D^+, CH^+...CH_4^+; Surface: clean, used, covered TS carbon tiles.

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Brief Report on the Activities within the Project: "Molecular Surface Interaction Dynamics" (RA No. 8607/CF)

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Surface dynamical calculations

Since 1995 we have studied molecular dissociation and atomic recombination at surfaces using a semiclassical computational technique, which quantizes phonon and electrons of the substrate whereas the atoms or molecules in the gas phase are treated using classical mechanics or quantum wave packet dynamics. The studies have shown that both phonon and electronic excitation in the substrate are of importance for sticking, energy accomodation and recombination processes. Work is presently being carried out which improves the description of electronic excitation in the solid.

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IAEA Co-ordinated Research Programme on
"Atomic & Plasma-Wall Interaction Data for Fusion Reactor Divertor Modelling"
Research Agreement No. 8681/CF

Final Report

Contracting Institution: Institute for Surface Modification e.V., Leipzig, Germany

Chief Scientific Investigator: Professor K. J. Snowdon

Period of Agreement: 01.08.1995 - 31.12.2000

Summary: The work performed for this CRP included:

1. Experiments in the laboratories of the chief scientific investigator on energy dissipation and molecular fragmentation in low energy molecule surface interactions [1,2,4,5,8].
2. Classical molecular dynamics simulations of low energy atom- and molecule-surface interactions, including exploration of molecular vibrational and rotational excitation and orientation and alignment effects [3,6].
3. Compilation of information from the literature on all known mechanisms leading to the ejection of low energy molecular species from surfaces [7,9,10].

This programme has resulted in 9 publications in refereed scientific journals and 2 reports in the NIFS-Data Series. Key results are provided in abstract form below.

Energy Dissipation & Molecular Fragmentation: This work has concentrated on obtaining a detailed understanding of the influence of local 'heating' of the metal substrate electron gas by fast moving molecular projectiles on the scattering and fragmentation distributions of such species [1,2,4,5,8]. At keV projectile energies, transfer of translational energy to the substrate via electron-hole pair excitation can be of the order of ~1 eV/Å of the fast particle trajectory in the surface region. The resulting 'hot electrons' are available to populate high lying projectile resonance's, which can lead to vibrational heating and eventual dissociation. The mechanism is particularly efficient under glancing incidence scattering conditions.

Molecular Dynamics Simulations: The rotational and vibrational distributions of fast diatomic molecules scattered from uncorrugated surfaces under strongly dissipative glancing incidence conditions have been calculated. The classical trajectory simulations include potential surface switching associated with hot-electron scattering processes. Both ro-vibrational excitation and strong alignment of the classical angular momentum vector in the surface plane ('cartwheel motion') were observed, independent of the occurrence of potential surface switching. Ro-vibrational excitation was strongly enhanced by transitions between potential surfaces. The resultant larger proportion of molecules in highly rotationally excited states leads to a higher fraction of cartwheel-aligned molecules in the scattered molecule ensemble. The molecules which dissociate in the simulation were characterised by surface normal peaked internuclear axis orientation distributions. This is in agreement with the results of recent experiments [2]. We observed in addition an enhanced rotational population of 'topspin' oriented molecules, which arose from differences in the surface parallel oriented friction forces acting on each atom of the molecule. We have also carefully compared molecular dynamics (MD) and binary collision approximation (BCA) scattering simulation codes for scattering of both light (He) and heavy (Xe) projectiles from a heavy target surface (Cu(111)) under glancing incidence

conditions [3]. We have demonstrated that use of the BCA leads to a wider range of scattering angles and overestimates the elastic energy losses. Furthermore, the BCA overestimates the importance of zig-zag trajectories in surface semi-channels.

Compilations: The mechanisms which may lead to the departure of molecular species from surfaces exposed to low energy (0.1 - 100 eV) particle or photon and electron irradiation have been reviewed in one invited article [7] and two research reports [9,10], all written in collaboration with Dr. H. Tawara and aided by financial support for KJS by NIFS. The processes which are likely to dominate under the conditions expected in gas-blanket type fusion reactor divertors are identified. The influence of the nature of the surface on the flux, ionised state, translational and internal energies of departing molecules are discussed. Particular emphasis was given to recombinative desorption mechanisms (especially Eley-Rideal) which have the potential to produce highly vibrationally excited molecular hydrogen. Such information may help guide the choice of appropriate materials and operating temperatures for plasma facing components of gas-blanket type divertors such as that recently proposed for the International Thermonuclear Experimental Reactor (ITER).

Copies of all publications relevant to the CRP are enclosed.

J. Stroud.

5-3-99.

List of Publications Relevant to the CRP

The following publications are related to and have been published within the period covered by the Agreement:

Refereed

1. Tzanev, A. Golichowski, W. Mix, K. J. Snowdon, Scattering of Fast N_2, N_2^+ and N_2^{2+} from Al(111) under Glancing Angles of Incidence, Surf. Sci. 331-333 (1995) 327-331
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International Atomic Energy Agency
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Arifov Institute of Electronics
Uzbek Academy of Sciences

Republic of Uzbekistan

Experimental and Theoretical Investigations of the Charge and Excitation States Formation Processes of Low Energy Atomic and Molecular Particles Outgoing the Solid Surface

(Progress Report for 1995/11/15-1998/11/14)

Principal Investigator

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I. INTRODUCTION

There were experimental investigations conducted in the framework of the Project in the Institute of Electronics during the period 1995-1998. These studies dealt with a series of inelastic processes that occur during a bombardment of solid surface by low energy particles.

A theoretic analysis of interaction processes of slow H_2 molecules and multicharged ions (MCI) with metal surfaces has been conducted. Studies related to an understanding of mechanisms of charged states formation of hyperthermal scattered and sputtered atoms have been performed, as well.

II. ESSENTIAL OBTAINED RESULTS

We have performed experimental determination of single scattered particles ionization degree η^+ in the energy range of 250 eV $\leq E_0 \leq$ 3000 eV for Ne and Ar atoms and 11 targets of V and VI periods. To conduct the analysis of neutrals they were preliminary ionized by electron impact. We found: within the limits of each period η^+ changes nonmonotonically; for the same group of elements $\eta^+_V > \eta^+_{VI}$; $\eta^+(E_0)$ increase more rapidly that can follow from Hangstrum formula $\eta^+ \sim \exp(-a/E_0^{1/2})$

The secondary ion mass-spectrum obtained under irradiation of graphite by Ne^+ and Ne^{2+} ions with the energy of E_0 = 500 eV was measured. There are present carbon ions C_n^+ type ($n \leq 3$), hydrocarbon ones C_nH_m ($m \leq 2$) and these of adsorbed gases H^+, H_2^+, O^+, H_2O^+, CO^+. It was founded that C_n^+ ions yield is independent of ion charge, but H^+, H_2^+ and CO^+ ions yield increases with charge increasing. Under H^+ ions bombardment practically the same spectrum was observed, but at E_0 = 18 keV n-value increases up to n = 19.

Mass-spectra and emission coefficients of positively charged ions sputtered as a result of bombardment of LiF and KCl surfaces by electrons with energy $10eV \leq E_0 \leq 1000eV$ have been measured by the SIMS method. It appeared that observed mass-spectra included several peaks corresponding to atomic ions: $Li^{Z+}, F^{Z+} (Z_{max} = 2)$ and $K^{Z+}, Cl^{Z+} (Z_{max} = 3)$ and molecular ions: $(KCL)^+, (LiF)^+, (Li_2F)^+$. The measurements showed that the threshold energies of sputtered single charged ions are determined by ionization energy of 3S inner shells of potassium ($\approx 37eV$) and 1S of lithium ($\approx 55eV$). An interatomic Auger transition transforms Cl^- and F^- into Cl^+ and F^+. The way this sputtering process arises is the Coloumb explosion of positively charged ions. An emission of multicharged and molecular ions is related to an ionization of deep levels of Cl and F by bombarding electrons. The threshold energies of these species are the same and correspond to the ionization energy of the 2P level of Cl ($\approx 240eV$) and 1S level of F ($\approx 636eV$). After that some multicharged and molecular ions appear as a result of a cascade of interatomic and interatomic Auger transitions.

Some measurements of coefficients of ion-electron emission γ under bombardment of Pt, Si, Be, LiF and NaCl by ions $Be^{Z+} (Z = 1 \div 4)$ with energy $250eV \leq E_0 \leq 4000eV$ as a function of energy and ion charge have been carried out. It is shown that the shape of the function $\gamma(E_0)$ strongly depends on the ion charge. In the case $Be^{Z+} \rightarrow LiF, KCl$ the conditions of existence of a potential emission are satisfied for $Z > 2$, only. Thus in the case when $Z = 1$ and $Z = 2$ only kinetic emission occurs, which implies $\gamma(E_0) \sim \sqrt{E_0}$ according to the existing theories, and in the case when $Z > 2$ both potential emission and kinetic one occur. The meaning of the obtained result is that γ_{kin} decreases quite rapidly as the ion charge increases and therefore one can disregard the contribution of γ_{kin} into γ when $Z = 4$ already. The physical cause of the observed phenomenon is related to the decrease in the cross-section of inelastic $Be^{Z+} \rightarrow$ LiF collisions with decreasing the number of electrons in the beryllium shells.

A low pressure high-frequent discharge into cylindrical geometry to obtain the atomic oxygen is used for a low-velocity flux and an external electrode usage. It has been shown that ion current density and positive ions energy are related to the middle range of positive pole of HF-discharge (p= 1-10 Pa, l = 150 cm, d = 5 mm, f = 30 MHz, P ~ 50-80 W). HF- plasma ion current density is $j = 10^{15}$ cm^{-2} s^{-2} for ions which have energy of about E_i = 5-10 eV.

It is obtained that atomic oxygen exposure (dose was about $3 \cdot 10^{21}$ cm^{-2}) can affect the loss of weight of pyrolitic graphite sample only slightly (about 1-3 %).

Computer simulation studies of processes of neutralization of slow MCI in the subsurface area of a metal leading to potential ion-electron emission and «hollow» atoms formation have been performed. A simulation of the processes of neutralization of MCI via resonance electron transition from the occupied part of a conduction band onto the high-excited levels has been included into software dealing with a calculation by Monte-Carlo method of cascades of Auger transitions. The calculations took into account a level promotion near the metal surface caused by image forces. By this code we have carried out calculations for the neutralization both of $Ar^{(10-18)+}$ on the gold surface and C^{6+} on the graphite surface.

From our calculations it follows, that at MCI's approaching the metal surface electrons have time to populate much deeper shells, than as it results from the solution of the rate equations. The results of calculations have shown that a significant part of neutralization energy can be transferred to electrons of the conduction band via both resonant loss of electrons into empty states of the conduction band and emission of captured electrons into vacuum by the promotion mechanism. As a result of the losing of the most of captured electrons via these two channels the MCI approach to the surface still being in charged states.

In the framework of model of formation of charged states of particles sputtered by primary knock-on, certain dependencies of an ionization degree of sputtered Ni and Be atoms on charge of the bombarding ions Ne^{Z+} and $He^{Z+}(Z = 1 \div 2)$ and on their energy $50eV \le E_0 \le 200eV$, have been computed. Rates of the electron exchange processes are taken into account in the model (Auger neutralization of bombarding and recoiling ions, relaxation of the excited area of the metal) were estimated with the help of published sources. It can be that in any case an ionization degree of Ni and Be atoms sputtered by double charged ions is higher than that of sputtered by single charged ions. The cause here is that the bigger is the ion charge, the more is the number of electrons from a local surface area spent on its neutralization and therefore the less electrons left available for neutralization of a sputtered ion.

The broadening of energy spectra of H atoms scattered by a metal surface under H_2^+, E_0 = (0,5 – 5) keV molecular ion bombardment was calculated taking into account the molecular ions to suffer dissociative neutralization on the initial part of their scattering trajectory. As a result of the neutralization the molecule atoms gain the repulsive energy in the center-of-mass system, that leads to the broadening of the energy spectra of the scattered atomic particles. Taking into consideration that molecules in the bombarding beam have an isotropic distribution over all molecular axes positions and using an analytical expression for the function describing the angle and energy distributions for the atomic scattering, the final distribution of scattered atoms over energies and scattering angles was calculated.The results also show the importance of the inelastic energy losses of the molecular constituents for their final energy distribution. The theoretical analysis indicate deviations from the Lindhard-Scharff approximation at low particle energies.

It was established experimentally that energy losses ΔE of hyperthermal (HT) *Xe*, *Kr* and *Ar* - atoms, scattered from *Ge*(100), *GaAs*(110) and *Ag*(110) surfaces can be well described by the following simple empirical formula: $\Delta E = k E_0 \cos^2\left((\theta_i + \theta_f)/2\right)$. Here E_0 is the energy of bombarding atom, θ_i and θ_f are the angles of incidence and emergence, k depends on the bombarding atom mass only. In the framework of the model of single elastic collision of incident atom with an effective mass, one can obtain the same expression for the ΔE.

The HT ion emission coefficient was represented in the following form:

$$Y^+ = Q \cdot S(E_0) \cdot P^+(E_0),$$

where $S(E_0)$ is the sputtering coefficient, Q is the atom coverage degree on the surface, $P^+(E_0)$ is the ionization probability.

In the case of K^+ ion emission from *Ag*-surface *K*-atom ionization potential (4.34 eV) is less than the *Ag*-surface work function (4.72 eV). So, virtually all sputtered potassium must escape from the surface as K^+ ions. This implies $P^+(E_0) \approx 1$ and $Y(E_0) \approx S(E_0)$. It was established that the function $Y_K(E_0)$ almost coincides with the function $S(E_0)$.

For In^+ ion emission the dependence $Y_{In}{}^+(E_0)$ was calculated by the formula with $P^+(E_0) = \exp(-v_0 / v_\perp)$, at $v_0 = 0.5 \cdot 10^6 cm/s$. This value of v_0 gives the correct absolute value of $Y^+(E_0)$ at $Q \approx 0.5$. The Hg^+ ionization coefficient at *Pt* surface bombardment by *Hg* atoms was calculated assuming that the Hg^+ ions are being formed preliminary by the ion emission of sputtered adsorbed *Hg* atoms. Under this assumption the calculation of $Y_{Hg}{}^+(E_0)$ function was performed. The absolute value of $Y^+ \approx 2 \cdot 10^{-6}$ was obtained at $Q \leq 10^{-2}$.

PUBLISHED PAPERS UNDER THE PROJECT

1995 – 1998

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1. Ferleger V. Kh., Medvedeva M.V., Wojciechowski I.A. The charge state of recoils under surface bombardment by multiple charge ions // Book of Abstracts of 11-th Int. Workshop on IISC, Germany, 1996, p.25.
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