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"ATOMIC, MOLECULAR AND PARTICLE-SURFACE INTERACTION DATA FOR DIVERTOR PHYSICS DESIGN STUDIES"

7-9 November, 1994, Vienna, Austria

SUMMARY REPORT

Prepared by R.K. Janev

July 1995

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

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ABSTRACT

The proceeding, conclusions and recommendations of the IAEA Advisory Group Meeting on "Atomic, Molecular and Particle-Surface Interaction Data for Divertor Physics Design Studies", held on November 7-9, 1994, at the IAEA Headquarters in Vienna, Austria, are summarized. The Advisory Group discussed in detail the present status of the atomic, molecular and particle-surface interaction data needed in the performance modeling of a dynamic gas target divertor, envisaged for the next-generation fusion reactors (such as ITER). The Group has identified the atomic and particle-surface interaction processes for which the present database is inadequate, as well as new classes of processes which should be included in the physics of divertor modeling codes. The scope of an IAEA Co-ordinated Research Programme, aimed at improving the required database, was formulated at the meeting, with a strong recommendation for its initiation in 1995.

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1. INTRODUCTION

In line with the recommendations of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council, given at the 7th Subcommittee meeting (October 16-17, 1992), the International Atomic Energy Agency convened on 7-9 November 1994, at its Headquarters in Vienna, Austria, an Advisory Group Meeting on "Atomic, Molecular (A+M) and Particle-Surface Interaction (PSI) Data for Divertor Physics Design Studies". The objectives of the meeting were:

(i) to review the status of A+M and PSI data currently used in the fusion reactor divertor modeling codes;

(ii) to identify new classes of A+M and PSI processes taking place in a cold and dense hydrogen plasma which should be included in the codes for improvement of their predictive power when modeling the divertor performance of next generation fusion reactors (such as ITER), and

(iii) to formulate the scope of an IAEA Co-ordinated Research Programme (CRP) aimed at improving the A+M and PSI data bases for fusion reactor divertor modeling.

The Meeting was attended by 12 participants and 3 observers from 9 countries and by the staff of the IAEA A+M Data Unit. The List of Meeting Participants is given in Appendix 1.

The critical review of atomic and particle-surface interaction physics content of divertor modeling codes became an urgent need with the recent proposal of a new, "dynamic gas target" concept for the ITER divertor. The new ITER divertor concept relies on a dominant role of atomic processes in the divertor region in exhausting the thermal plasma power (of the order of 300 MW in ITER) and envisages divertor plasma temperatures as low as about 1eV (near divertor plates) and neutral particle (atomic and molecular hydrogen) densities up to 10^{15} cm^{-3} in the cold divertor regions. The main trust for the plasma energy exhaust is placed on plasma edge impurities, while for the plasma momentum dispersion over the divertor walls the elastic and momentum transfer ion-neutral collisions are considered critical.

Under such plasma temperature and neutral density conditions, whole classes of atomic, molecular and particle-surface processes become important for the plasma and neutral gas kinetics, energy and particle balance and transport, and for other aspects of plasma behaviour. Many of these processes, considered previously less important, are not adequately (or at all) represented in the existing divertor modeling codes. Examples are the processes involving vibrationally excited molecules and molecular ions, the exothermic ion-molecule reactions,

molecule formation or dissociation processes on surfaces, and some others.

During the meeting preparation stage, the potential meeting participants were asked to prepare compilations and critical reviews of the available data for certain classes of gas-phase and particle-surface atomic collision processes, while the expected meeting participants from the divertor modeling community were asked to perform selected runs of their modeling codes to test the sensitivity of certain code results (for some global divertor plasma/neutral gas properties) to the effects introduced by the new classes of processes. It should be emphasized that all meeting participants have done an excellent and extensive preparatory work, what contributed significantly to the meeting efficiency and results.

2. MEETING PROCEEDINGS

After the opening address and adoption of the meeting agenda (see Appendix 2) the work of the meeting proceeded in the following six sessions:

Session 1: Modeling of edge/divertor and similar low-temperature plasmas,

Session 2: Electron-impact processes,

Session 3: Heavy particle collision processes,

Session 4: Particle-surface collisions,

Session 5: Presence and role of vibrationally excited molecules, H^- and H_3^+ in the plasma edge,

Session 6: Scope of an IAEA CRP on A+M and PSI data for fusion reactor divertor modeling.

Three comprehensive review talks were presented during the first meeting session. Dr. D. Reiter (IPP-Jülich) provided an exhaustive account of the present A+M and PSI data content of divertor modeling codes. He first briefly discussed the main physical ideas on which the new "dynamic gas target" concept for the ITER divertor is based and the new atomic and particle-surface interaction physics involved in this concept. Then, Dr. Reiter outlined the currently used A+M and PSI data information in the most advanced divertor modeling codes (such as EIRENE and DEGAS for the neutral particle transport, and B2 for the plasma transport) and emphasized the needs for upgrading this information to cover the multitude of A+M and PSI processes occurring in a very low temperature and high neutral density divertor plasma ($1eV \lesssim T < 10eV$), presently not included in the divertor modeling codes. Dr. Reiter provided a number of code results with assumed cross sections for three groups of vibrationally excited molecules, demonstrating that under certain plasma conditions (or in certain divertor plasma regions) the role

of the processes of vibrationally excited molecules may be important (e.g. for the power exhaust).

During the same meeting session Dr. M. Bacal (Ecole Polytechnique-Palaiseau) reviewed the current knowledge on the atomic, molecular and surface processes in low-temperature hydrogen plasma of H^- sources with emphasis on the relevance of this information for the divertor plasma kinetics. Dr. Bacal focussed her presentation on those processes which could potentially be instrumental for a rapid volume recombination of the plasma electrons and ions. According to the experience with other low-temperature hydrogen plasma (H^--sources, plasma jets of cascaded arcs), the main volume recombination channels include reaction chains leading to formation of H^-, H_2^+ and H_3^+ ions which then recombine rapidly with the plasma protons and electrons, respectively. She stressed the crucial role of the collisions of vibrationally excited H_2 molecules and of the H_2 molecules in high Rydberg states in the formation of H^-. Dr. Bacal also reviewed the particle-surface collisions in the plasmas of H^- ion sources and emphasized the potential role of these collisions in forming vibrationally excited H_2.

In an in-depth presentation, Prof. M. Capitelli (University of Bari) provided a thorough overview of the kinetics of low-temperature hydrogen plasmas (including the particle-surface interaction processes) and addressed the question of the vibrational population distribution of H_2 in such plasmas. Within a plasma neutral gas kinetics model, which solves simultaneously the master equations for the vibrational kinetics and the Boltzmann equation for the electron energy distribution function, and includes the positive and negative ion kinetics, the dissociation kinetics and a number of atom (molecule)-surface process, it was found that for conditions typical for an H^- source non-equilibrium plasma the vibrational distribution of the H_2 molecules saturates already at the levels with vibrational quantum numbers v=4-5. With respect to the v=0 level population, the population of $v \geq 5$ is about five orders of magnitude smaller. (However, the rate coefficient for electron attachment on these molecules increases by approximately the same factor with respect to its value for the v=0 state, facilitating thus the formation of H^- ions in these types of plasmas).

In the meeting session on electron-impact processes in divertor-type plasmas six comprehensive data collections for various electron-atom and electron-molecule collision processes were presented. Prof. J.M. Wadehra (Wayne State University - Detroit) presented an extensive overview of the cross sections for all electron-impact (elastic and inelastic) processes of H and H_2 (and its isotopic variants), including the processes with (ro-)vibrationally excited H_2. Special emphasis was given to the processes of electron attachment to (ro-)vibrationally excited

H_2 and to the processes of vibrational excitation of H_2 through the intermediary H_2^- (X) resonant state and to the dissociative excitation of H_2 (through the intermediary H_2^* (b) state). Prof. Wadehra addressed also the question of the scaling of the cross sections for some of the considered processes with respect to the initial vibrational (or rotational) quantum number and with respect to the mass of the hydrogenic isotope.

Prof. J.B.A. Mitchell (University of Western Ontario-London/Canada) presented on exhaustive review on the electron-molecular ion collision processes, including the hydrogenic ions H_2^+, H_3^+ and their isotopic variants, and the O_2^+ and CO^+ ions. The processes considered included: dissociative recombination (also for individual ro-vibrational states of the ions), dissociative excitation and ionization, and ion-pair formation. Apart from presenting the cross sections for these processes in the considered systems (including the most recent experimental and theoretical results), Prof. Mitchell also provided information on the vibrational level populations of the ions resulting from different modes of their production. He also analyzed the effects of (ro-)vibrational excitation of the ions on the cross section magnitudes of various processes.

Prof. T. Fujimoto (Kyoto University) presented the elements of a collisional-radiative (CR) model for molecular hydrogen. The model includes explicitly all the electron-impact processes of H_2 up to the molecular electronic states which in the dissociation limit correspond to $n \leq 2$ atomic states, and the processes involving higher molecular excited states are included in the model by using suitable cross section scaling relationships. The electron-impact excitation, ionization and recombination processes are considered (including their dissociative channels), as well as the radiative processes. The processes involving vibrationally excited H_2 are, however, not included in the model. Prof. Fujimoto presented a detailed account of the cross sections used in his CR model as well as numerous results on the effective CR rates for ionization, recombination, neutral atom formation, etc. He also presented the results of this model for electron energy and radiative losses for a broad range of plasma parameters. In addition, Prof. Fujimoto presented examples of vibrational-level population distributions for the ground state of H_2 and modifications incurred to the above effective CR rates.

Dr. R. Celiberto (Universita di Bari) presented the results of the quantal calculations (performed jointly with Profs. M. Capitelli and U. Lamanna) on electron impact excitation of H_2 (v_i;X) (v_i=0-14) and D_2 (v_i;X) (v_i=0-20) to the excited (v_f;B) and (v_f;C) states of these molecules, v_i and v_f being the initial and final state vibrational quantum numbers. Cross sections were

presented both for individual $v_i \rightarrow v_f$ transitions and for the total excitation from a given initial state v_i. The energy range covered by these calculations was from threshold to 200 eV. In addition, Dr. Celiberto presented cross sections (in the same energy range) also for the electron-impact induced dissociation in the continuum of the B and C excited states.

Dr. T. Kato (NIFS-Nagoya) presented the collisional database for and the results of a collisional-radiative model for carbon atoms in a plasma. She showed a large collection of critically assessed excitation data for the states with principal quantum number up to n=4. The model also includes the ionization and recombination (RR and DR) cross sections (or/and rates) for all the individual states included in the model. The quantities computed by the model for a wide range of plasma temperatures and densities were: effective ionization and recombination rates, effective emission rate coefficients and the line radiation power coefficient.

Prof. T. Fujimoto (Kyoto University) reviewed the recent developments in the collisional database for the collision-radiative (CR) model of helium. Since his first compilation of the cross section for the collision processes involved in the CR model of helium in 1979, there has been much (both experimental and theoretical) work devoted to electron-helium atom (and ion) collisions, which resulted in a significant improvement of the collisional database for the processes involving the excited helium states. The results on the effective CR-rates, however, seem to be little affected by these changes in the database, except in a few cases.

The cross section information on the most important heavy particle collision processes in low-temperature divertor plasmas was presented during the 3rd meeting session in five reports. Dr. D.R. Schultz (ORNL - Oak Ridge) presented new calculations for the elastic, momentum transfer, viscosity and charge exchange cross sections for the basic ion-atom and atom-atom collision systems in a divertor plasma (H^+, He^+, He^{2+}, H^-, H, He and their isotopic variants). The covered collision energy range was 10^{-3} - 10^2 eV. Dr. Schultz described the method used in these calculations and made comparison with the results of other authors. Analytic fits were provided for all calculated cross sections in a format suitable for use in the plasma modeling codes.

Prof. F. Brouillard (Université Catholique de Louvain, Louvain-la-Neuve) gave an exhaustive overview of the available cross sections for rearrangement process in low-energy (below 10 keV - C.M.) collisions involving neutral and ionized hydrogen and helium atoms, hydrogen molecules and their ions, and hydrogen negative ions. The particle rearrangement processes included electron transfer, ionization, detachment, dissociative and associative processes

and Penning ionization. The systematic and comparative presentation of the cross sections for all these processes provided a possibility to assess their relative importance at various energies. Dr. R.K. Janev (IAEA) provided a similar critical evaluation of the available cross sections for the particle-interchange reactions in hydrogenic (including isotopes) and helium ion-molecule collision systems. Particular attention was given to the exothermic reactions and the effect of internal energy state of the reactants on the reaction cross sections. The energy region covered by this analysis (performed in collaboration with Prof. F. Linder, University of Kaiserslautern, and Dr. J. Botero, IAEA) was the one below ~ 10 eV - C.M., where the cross sections of the considered reactions (when exothermic) are large. The subject of low-energy heavy-particle reactions was further elaborated by Dr. H. Tawara (NIFS-Nagoya) who presented a comprehensive overview of all important types of plasma edge relevant reactions including ro-vibrational excitation, dissociative excitation, ionization and charge transfer, and chemical (atom and proton transfer) reactions. Dr. Tawara also emphasized the important role that internal energy state of the reactants plays in the reaction dynamics. In the last presentation of this Session Dr. V. Abramov discussed the role of low-energy charge exchange processes in the new ITER divertor concept and the data needed for these processes for the divertor modeling codes. Dr. Abramov analyzed the accuracy of several sets of charge exchange data in the context of their effects on modeling code results.

The fourth session of the meeting was devoted to particle-surface interaction processes. Three presentations were given during this session. Prof. K. Snowdon (Universität Osnabrück) reviewed the basic low-energy mechanisms of atom (ion, molecule) - surface interactions leading either to formation or dissociation of molecules (or their ions). Prof. Snowdon also presented the available experimental and theoretical information on these processes paying particular attention to the charge and quantum (including vibrational) state distribution of reaction products, as well as their energy and angular distribution. While there is now a (relatively) good understanding of the physical mechanisms of various low-energy particle-surface processes leading to molecule formation or destruction, the available information on their quantitative characteristics for the energy range (1-100 eV) and surfaces of direct fusion interest is still extremely sparce. Dr. R. Heeren (FOM AMOLF - Amsterdam) presented the recent results in the field of negative hydrogen ion formation on surfaces upon impact of H_n^+ (n=1-3), C^+ and O^+. The presented results were mainly those obtained by the FOM Institute in Amsterdam on tungsten and silver surfaces, covered by Cs or Ba (mono)layers, and the energy range covered was 100 eV-1000 eV.

It was shown that on a Ba surface the conversion of incident positive H_n^+ ions into "reflected" $H^-(D^-)$ ions could be as high as 5-7%. Prof. E.W. Thomas (Georgia Tech.-Atlanta) provided a comprehensive review of the existing databases for particle reflection, physical sputtering and (secondary) electron ejection in particle-surface interaction. Prof. Thomas emphasized the inter-relation between all the considered processes (through the common underlying physics - the multiple scattering process, and even a common dynamical parameter - the electronic stopping power) and, with this in mind, he made an inter-comparison of their coefficients (yields) for a number of material surfaces of fusion interest.

In Session 5, the meeting participants discussed the overall status of the A+M and PSI databases for divertor modeling, taking particularly into account the physical conditions in a "dynamic gas target" type divertor as has been proposed for ITER. Special attention was given to the data needs for accurate modeling of the plasma energy exhaust by the neutral hydrogen-helium gas in the divertor, and in particular to the data information for the processes involved in the volume recombination of the plasma. Provided the divertor plasma temperature is sufficiently low (around and below 1 eV) two basic mechanisms were identified as major contributors to the volume recombination: dissociative electron attachment to electronically or vibrationally highly excited H_2 molecules with subsequest H^+ - H^- recombination (to form a radiating H(n=3) atom), and atomic-to-molecular ion conversion (H^+ to H_2^+ or H_3^+) via exothermic particle-interchange ion-molecule reactions with a subsequent electron (dissociative) recombination on H_2^+ or H_3^+. Since in both recombination mechanisms the chains of reactions involved require vibrationally excited H_2, much of the discussion was devoted on the mechanisms of formation of H_2 in highly vibrationally excited states ($v \geq 4$) and on the question of vibrational level populations of $H_2(v)$ in a ITER divertor type plasma. Several participants referred to the recent experimental evidence about formation of H_2 in highly vibrational states on surfaces via the Eley-Rideal mechanism. Prof. Capitelli showed new results on the $H_2(v)$ vibrational level population obtained by his group in Bari by taking into account all the necessary level population and destruction processes in a plasma with parameters not much different from those of a divertor plasma. These results have indicated that the vibrational population saturates for $v \geq 4$ on a value about 10^{-4} times lower than the population of the v=0 level. In the negative ion source plasmas, such populations are sufficient to ensure significant negative ion production via the dissociative electron attachment. The electron or atom exchange reaction in the $H^+ + H_2$ system would also be greatly enhanced if H_2 is vibrationally excited in states with $v \geq 4$. The created

H_2^+ ions in these reactions would (dominantly) recombine (dissociatively) with plasma electrons if temperature is below ~ 1 eV, but they would (dominantly) dissociate under electron impact if plasma temperature is above ~ 2 eV. Formation of H_3^+ ions in $H_2^+ + H_2$ collisions is unlikely in the temperature range above 0.1 eV since its reaction rate coefficient is about two orders of magnitude smaller than those for $e + H_2^+$ recombination (below T_e ~ 1.5 eV). (The H_3^+ formation and electron-impact H_2^+ removal rates would become comparable if the H_2 density is correspondingly higher than the electron density to compensate for the difference in reaction rate coefficients).

The meeting participants discussed also other possible mechanisms for enhancing the volume recombination of a divertor plasma. Prof. Mitchell brought attention to the fact that the direct radiative electron-proton recombination can be enhanced by several orders of magnitude in the presence of strong external electromagnetic fields of suitable frequencies (photon stimulated radiative recombination). He also noted that the ion-interchange reactions of H_2^+ (v) with He and Ne are exothermic for $v \geq 2$ and $v \geq 1$, respectively, and their products HeH^+ and NeH^+ in collisions with H_2 could lead to formation of H_3^+. In order to estimate the efficiency of this reaction chain, one should know the destruction rates of HeH^+ by electron impact (dissociative excitation and dissociative recombination). The conclusions of the discussions in this session, as well as the consequent recommendations regarding the possible actions that the Agency could undertake to contribute in improving the A+M and PSI data for divertor plasma modeling, are given in the next section of this Report.

The last session of the Meeting was devoted to discussion of the scope of a Co-ordinated Research Programme (CRP) that the Agency could undertake as one of the measures for improving the divertor plasma modeling A+M and PSI databases. Both the content and the potential participants of the suggested CRP were discussed. At the end of this session the participants also discussed and adopted the Meeting conclusions and recommendations.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS*

3.1. Meeting Conclusions

A. General

1) The collisional kinetics of a divertor plasma with temperatures below 10 eV is substantially different than that of a plasma with temperatures above 10 eV. This is a consequence of differences in reaction rate coefficients for various collision processes in the two temperature regions. While for $T_e > 5$ eV, the hydrogenic plasma is in an ionizing regime, for $T_e < 2$ eV the plasma is in a recombining regime. Consequently, both the plasma composition (relative ratio of ionized to neutral particles) and the dominant collision processes are different in the two temperature regions. Similar differences exist also in the particle-surface interaction processes: at higher temperatures the plasma particles have sufficiently high mean energy to penetrate into the first-wall material and induce multiple-collision (cascade) particle emission effects, while at low temperatures the collision dynamics (or chemistry) on the surface determines the result of the collision event.

2) From the point of view of data availability, the cross section database for the processes involved in the modeling of divertor plasmas with temperatures above 5-10 eV is much better documented than the database for the processes in divertor plasmas below 5-10 eV. In the low-temperature regime, a significant part of the plasma energy may be stored in the vibrational modes of the molecular gas and, therefore, all processes involving vibrationally excited molecular species (neutral and ionized) become very important. The database for such processes is rather incomplete, and is based mainly on theoretical computations, sometimes performed with crude models. The quantitative information on low-energy particle-surface processes for the candidate divertor wall and divertor plate materials is virtually non-existent. However, the knowledge on the basic mechanisms for these processes is significant and the experimental and theoretical methods for their study are well established.

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* Written comments for this part of the Report were obtained from Profs. M. Bacal, J.B.A. Mitchell, T. Fujimoto, E.W. Thomas, K. Snowdon and M. Capitelli. These comments have been incorporated in this section within an appropriate context.

3) Although highly sophisticated and powerful in their potential, the codes presently used for modeling the divertor performance still do not include important parts of the atomic, molecular and particle-surface interaction physics of the "dynamic gas target" divertor. This is particularly true for the plasma temperature regimes below 5 eV and neutral particle-densities above 10^{15} cm^{-3}. Improvement of the predictive power of the codes for the low-temperature, high-neutral-density divertor plasma conditions would require significant new atomic physics and particle-surface interaction input. Inclusion of all the new physics in the codes in a direct way (e.g. by treating the excited electronic and vibrational state individually) would increase the complexity of the codes and the required computing time (e.g. of the codes base on the Monte Carlo techniques) beyond the practically reasonable limits. Therefore, introduction of effective reaction rate coefficients (by prior solution of the corresponding "collisional-radiative" type problems for certain divertor species, such as molecular hydrogen, helium etc) to account for the effects of multistep processes would be a possible approach for simplifying the collisional kinetics. Another possibility would be a multi-group approach to the excited-particle spectrum with effective rates for each particle group. In both approaches, however, information on the complete matrix of reaction rate coefficients (i.e. for all states) would be required.

4) The Meeting discussions and analyses lead to the conclusion that the enhancement of volume recombination of plasma electrons and ions (with respect to the basic collisional-radiative recombination) in the temperature region 0.1 - 2 eV is possible basically through two mechanisms: 1) dissociative electron attachment to vibrationally excited molecules ($v \geq 4$) followed by recombination of produced negative ion with low-energy plasma protons, and 2) plasma ion conversion (on H_2) into a molecular ion (H_2^+) followed by dissociative (e - H_2^+) recombination. For comparable plasma and neutral gas densities the ion-ion recombination is the only effective recombination mechanism which can operate if the plasma temperature is below ~ 1 eV). (The role of the ion-conversion mechanism at such densities is about two orders of magnitude smaller than that of the dissociative electron attachment on H_2 ($n \geq 4$) molecules). For molecular hydrogen densities about one order of magnitude (or greater) higher the electron plasma density, the ion conversion mechanism becomes also important (for plasma temperatures below ~ 2 eV), particularly for the vibrationally excited molecular fraction, H($v \geq 4$). For $T \leq 1.5$ eV both the $H^+ + H_2 \rightarrow H_2^+$ production reaction is faster than the competing $e + H_2 \rightarrow 2\ H$ dissociation,

and the $e + H_2^+ \rightarrow H + H^*$ dissociative recombination is faster than the competing $e + H_2^+ \rightarrow e + H^+ + H$ dissociation. For still higher H_2 densities (about two orders of magnitude higher than the electron density) the rate of H_3^+ formation in $H_2^+ + H_2$ collisions starts to compete with the rate of $e + H_2^+$ recombination, and the recombination process $e + H_3^+ \rightarrow 3H$ ($E < 1$ eV) or $H_2(v \geq 4) + H^*(n = 2)$ ($E > 1$eV) becomes important. It should be noted that in all dissociative recombination processes (as well as in the exothermic particle-interchange reactions) the neutral products carry kinetic energies of several eVs (i.e. there is a neutral gas heating effect).

The effectiveness of impurity atoms such as He or Ne in converting H_2^+ into H_3^+ (via two steps), or in depleting the $v > 2$ levels of $H_2^+(v)$ ion (due to exothermicity of corresponding particle-interchange reactions for these levels), is in proportion with their concentration ratio with H_2. If there is a mechanism in the plasma for populating effectively high Rydberg states of H_2 (H_2^{**}), that would significantly enhance the plasma recombination by two reaction chains: i) dissociative electron attachment (with a rate coefficient of the order of 10^{-6} cm^3/s for $T < 1$ eV) with consequent $H^- + H^+$ mutual neutralization, and ii) charge exchange with protons, i.e. $H_2^{**} + H^+ \rightarrow H_2^+(v) + H^*(n)$ (with a rate coefficient of the order of 10^{-6} cm^3/s for $T < 100$ eV) with a consequent dissociation of $H_2^+(v)$ for $T > 1.5$ eV or dissociative recombination with electrons for $T < 1.5$ eV. However, unless created by a multistep mechanism, the direct electron-impact excitation of high Rydberg states of H_2 requires electron energies above 20 eV. The proton neutralization by charge exchange with H_2^{**} in the temperature region $T \gtrsim 20$ eV will, therefore, be immediately compensated by proton production in the electron-impact dissociation of H_2^+, the other product of the $H^+ + H_2^*$ charge exchange reaction.

5) Enhanced volume plasma recombination in the temperature range $0.1 \text{ eV} < T \lesssim 2$ eV evidently relies on existence of a substantial fraction of H_2 molecules in vibrational states with $v \geq 4$ and on high H_2 densities. The most important known mechanisms for formation of H_2 ($v \geq 4$) are the proton-impact vibrational excitation, effective in the temperature range ~ 10-100 eV (with a reaction rate coefficient of ~ 10^{-8} cm^3/s), the electron-impact excitation of $B\ ^1\Sigma$ and $C\ ^1\Pi$ electronic states of H_2 (effective for $T > 15$-20) followed by their rapid radiative decay to $X^1\Sigma$ ground state (in vibrationally excited states with $v \geq 4$) and the atom-impact surface recombination (Eley-Rideal) mechanism. (Over-Boltzmannian population in $H_2(v)$ produced on the surface via the Langmuir -

Hinshelwood mechanism is also possible but mainly for $v \leq 3$). Of all these three major mechanisms, only the Eley-Rideal mechanism does not require plasma temperatures above 10-20 eV. The vibrationally excited molecules are subject to many interaction processes with plasma particles, neutral gas particles and with the divertor walls (usually with increased cross sections), and the final vibrational level population is determined by a complex collisional kinetics with non-Maxwellian particle energy distributions. The solution of the volume plasma recombination problem has to be, in principle, solved simultaneously with the vibrational level population problem. This indicates the size of the required atomic and particle-surface interaction database for an accurate description of the volume plasma recombination.

6) From the point of view of modelling the plasma power exhaust in the divertor region, the class of participating processes is much wider. The correct estimate of the contribution of the neutral hydrogen and helium to the power exhaust in the divertor includes all the processes between plasma electrons and protons and the hydrogen and helium neutrals and ions. This means that not only the relevant collisional-radiative (CR) models for atomic hydrogen, molecular hydrogen and helium have to be constructed, but that they have to be also mutually coupled and considered in a self-consistent way. Only the CR model for atomic hydrogen can presently be considered as well established. Rough estimates with the available database indicate that the hydrogen and helium cannot extract more than 20-30% of the plasma power and that the main trust in plasma power exhaust should be put on plasma impurities.

   However, the interaction of ionized plasma impurities with the high-density neutral hydrogen in the divertor (e.g. via charge exchange) establishes a strong coupling between the power exhaust by hydrogen and impurities, and the whole power exhaust problem has to be treated self-consistently. This fact further expands the required atomic database for divertor modelling.

B. Data Status and Needs

B.1. Electron-atom and electron-molecule collisions

1) The electron-impact database for atomic hydrogen (including processes with excited states) can presently be considered as well established. For the processes in the lower

part of the level spectrum there is good agreement between the experimental and theoretical data. For the processes in the upper part of the level spectrum, the theoretical predictions (e.g. scalings) should have sufficient accuracy.

2) The electron-impact processes involving ground state hydrogen molecules and molecular ions are, generally speaking, also well documented. The main uncertainties and gaps in this database exist for the processes involving vibrationally excited states. Although there already exist a large number of calculations for these processes (e.g. for dissociative attachment, excitation to the lower bound and dissociative electronic states, direct dissociative ionization, dissociative recombination, etc), many of these calculations have been performed involving crude models for some parts of the collision dynamics. Full quantum-mechanical treatment (at least of the electronic motion) and extension of these calculations to higher electronic (bound and dissociative) molecular states is required. Search of appropriate cross section scaling relationships (with respect to the initial vibrational state, isotopic mass, and other collision or system parameters) should be pursued in order to reduce the size of the required computational effort and to achieve a more compact presentation of the data information.

   For the electron-impact induced transitions between the ro-vibrational states in the ground electronic configuration, the available theoretical models provide sufficiently accurate predictions.

3) The cross section database for electron-helium atom collisions is well established only for transitions from the ground state. Although data are available almost for all transitions between the states with n=2-4, there exist large uncertainties (a factor of five, or more) in some cases (even for optically allowed transitions). The main uncertainties are for the spin-forbidden transition in the energy range of the cross section maximum. For the transitions to and between the states with principal quantum numbers $n \geq 5$, the available scaling relationships should be able to provide sufficiently accurate cross section information.

B.2. Heavy-particle collisions

1) The most important heavy-particle processes in a "dynamic gas target" divertor are those related to the plasma momentum exhaust (ion-neutral and neutral-neutral elastic and momentum transfer collisions), energy and particle transfer (ro-vibrational excitation,

particle-interchange reactions) and charge exchange (electron capture) processes.

2) Establishment of systematic databases for elastic, momentum transfer and viscosity cross sections in ion-neutral and neutral-neutral collisions has been initiated recently in several laboratories and a significant amount of data has already been generated (mainly for the simple systems involving hydrogenic ions and neutrals and helium). The semi-classical approximation has proved to be able to provide quite accurate results for these processes in the energy region below 100 eV, provided the interaction potentials are known with sufficient (fairly high!) accuracy. Computational codes based on the semi-classical approximation are presently available in several laboratories. A more complex channel-coupling formalism (using a molecular basis) will be necessary to employ for generation of elastic and momentum transfer cross sections when the collision energy or the collision systems are such that the coupling of elastic and inelastic channels becomes strong (i.e. at higher energies and for ions in higher (than one) charge states).

3) Proton (ion)-impact induced ro-vibrational excitation of molecular hydrogen is an important process in the energy range 10-100 eV, but still not adequately well studied. Information is lacking particularly for the proton (ion) induced v-v transitions. The cross section information for v-v processes in hydrogen atom-molecule collisions has become available recently for energies below 10 eV.

   The energy transfer ion-molecule reactions below ~ 50 eV are strongly coupled with the particle-interchange and electron capture reaction channels, which imposes high requirements on the theoretical models. Presently, there exist well elaborated theoretical methods (such as the Infinite Order Sudden Approximation - IOSA) which can ensure adequate description of all coupled channels in the discrete spectrum. These models have so far been applied, however, only to the simplest ion-molecule systems and have not included the dissociation channels. In general, the available information on the energy transfer, particle interchange and electron transfer reactions in ion-molecule systems is very limited, particularly when the molecules are in vibrationally excited states.

4) The electron transfer processes in impurity ion-hydrogen atom (or molecule) collision systems have increasingly (with the ionic charge) large cross sections in the energy region below 100-200 eV. Even for single charged ions, the electron capture cross section becomes significant in the region below several eV due to the polarization

capture (Langevin) mechanism. For the common fusion plasma impurities (C, O, Be, B, Fe ...) the experimental charge exchange cross section data for the H, He and H_2 targets are extremely sparce in the low energy region (below e.g. 50 eV). While certain simple theoretical models can be used for fair estimates of the total electron capture cross sections for ions with $q \geq 3$, for the ions with q=1,2 and for determination of final state population in these reaction, semiclassical (for E > 100 eV) and quantal (for E < 100 eV) molecular-orbital coupled channel calculations are required.

The electron rearrangement processes involving hydrogen and helium ions and atoms (even in excited states) in the energy range above 100 eV have been extensively studied both experimentally and theoretically, and the corresponding cross section database is in relatively good shape.

B.3. Particle-Surface Collision Processes

1) The low-energy particle-surface interaction physics is presently fairly well understood but quantitative information on the specific processes involving divertor plasma constituents and candidate divertor wall and plate materials in the collision energy range of interest (~ 0.5 - 100 eV) is extremely sparce. Vibrationally excited H_2 molecules can arise via prompt desorption of H_2 formed in exothermic surface recombination reactions of adsorbed or implanted H-atoms (L-H mechanism), or in abstraction reactions of impinging H-atoms or hydrogen containing species (E-R mechanisms). The relative importance of these processes with respect to other possible processes which affect the near-surface molecular hydrogen density (e.g. sticking, reflection, adsorption, thermal or particle-impact induced non-associative desorption, etc) should be investigated for various incident energies, types of surfaces and surface conditions (cleanness, roughness, temperature, etc). There already exist well developed experimental and theoretical methods for undertaking such studies.

2) Low-energy (E < 2 eV) protons, after being neutralized at large distances from the surface, may recombine with adsorbed surface atoms via the E-R mechanism and form vibrationally excited H_2 molecules. The molecular H_2^+ and H_3^+ ions presumably undergo charge transfer in slow collisions with surfaces. Dissociative charge transfer my produce excited atomic and molecular (in the case of H_3^+ ions) products, while charge transfer to the ground electronic state of H_2 may be accompanied by significant

vibrational excitation.

3) Negative hydrogen ion formation in collisions of slow atomic and molecular hydrogen ions with surfaces has also been demonstrated, provided the surface work function is sufficiently low. $H^-(D^-)$ formation on Be surfaces has not been investigated but could be significant.

4) The information on the effectiveness of other surface processes, such as electron and photon induced desorption, sticking, direct (potential) reflection, resonant and Auger neutralization or ionization processes, for the surfaces of candidate divertor wall (and plate) materials is also very limited. The information on particle (and energy) reflection coefficients generated by the existing codes based on the classical collision dynamics (TRIM, MARLOWE, molecular dynamic codes) should be taken with reservations for collision energies below ~ 10 eV (where the quantum effects are dominant). In the 10-50 eV energy range the results of molecular dynamics codes should be preferred over those of TRIM, MARLOWE, BABOUM etc., provided the interaction potentials of the considered collision systems are determined accurately.

5) The information on particle surface processes should include not only their effectiveness (rate, probability, etc) but also differential characteristics, such as energy and angular distribution of reaction products, dependence on initial collision parameters (impact energy, angle of incidence), and for certain processes also specification of the quantum states of the products.

C. Needs for and Scope of an International, IAEA Co-ordinated Research Programme for Improving the Atomic and Particle-Surface Interaction Data Base of Divertor Modelling

1) The conclusions presented in sections A and B above show that the presently available data information on atomic, molecular and particle surface interaction processes in a "dynamic gas target" divertor, as proposed for the next-generation fusion tokamak devices (such as ITER), is by far insufficient for a successful (predictive) modelling of the divertor performance with respect to both power and particle exhaust, as well as with respect to its other operational features (impurity control, pumping characteristics, wall erosion, etc). The firm establishment of the conditions for an effective radiative power exhaust from the divertor region and for creation of a "detached" plasma in the near divertor plate region (through rapid volume recombination and other atomic plasma

energy and momentum loss processes) requires an in-depth and accurate knowledge of the collisional and radiative characteristics of a large number of atomic and particles-surface interaction processes. Many of these processes are presently not included in the divertor modelling codes, nor the data information for them is available.

2) The priority in the new data generation and in the collection and critical assessment of available data (if not already contained in the existing databases) for the standard divertor plasma constituents and in the energy range 0.1-200 eV should be given to the following processes:
   (a) all electron-molecule (molecular ion) collision process involving both ground and excited (electronic and vibrational) states;
   (b) all ion-neutral and neutral-neutral elastic and momentum transfer processes;
   (c) all ion(atom)-molecule processes involving energy exchange (ro-vibrational transitions) or particle rearrangement (electron capture, heavy particle interchange), including the dissociative channels and vibrationally excited molecular states;
   (d) all electron capture, particle interchange and energy transfer processes between plasma impurity ions and hydrogenic neutrals;
   (e) all particle-surface interaction processes leading to molecular (molecular ions) formation, destruction, vibrational deactivation, ion formation or neutralization, particle adsorption (sticking) and desorption (including thermal and particle-impact induced modes) and particle reflection (and retention).

   The information required on the above processes should include, apart from the integral, also their differential characteristics, such as energy and angular distributions of the products, quantum state characterization of reaction products (final state distributions) etc.

3) Efficient generation of the required information for improving the atomic and particle-surface interaction physics of divertor modelling codes is only possible through a co-ordinated international effort which would integrate the expertise and data generation capabilities of various highly specialized theoretical and experimental research groups from the relevant parts of the physics community. Some of the national Atomic and Molecular Data Centres for Fusion should also be involved in this effort (for data collection and processing). Strong interaction of this group of experts with the fusion divertor physics community and direct involvement of divertor plasma modelers in this international effort are also necessary to ensure the required focussing and implementation

of the data into modelling codes. The IAEA, through its atomic and plasma-material interaction programmes for fusion, is technically well prepared to undertake the co-ordination of this international effort.

3.2. Meeting Recommendations

1) The Advisory Group finds that, in order to adequately describe the physics of "dynamic gas target" divertors and improve the predictive power of divertor modelling codes, it is necessary to extend the atomic and particle-surface interaction database of the codes by inclusion of the low-energy processes discussed in the preceding parts of this Section.
2) The generation of the required data for improving the atomic and particle-surface interaction database of divertor modelling codes should be conducted in a co-ordinated manner to achieve high efficiency and better focussing of the effort. Close collaboration between the data users (fusion community), data producers (atomic and surface science communities) and the international atomic data centre network for fusion should be established.
3) It is strongly recommended that the IAEA undertakes a Co-ordinated Research Programme (CRP) on the subject of atomic and particle-surface interaction data for divertor performance modelling, which should include the collection, generation and implementation into the modelling codes of the required data. The scope of this CRP has been outlined in the preceding part of this Section.

Appendix 1

IAEA Advisory Group Meeting on "Atomic, Molecular and Particle-Surface Interaction Data for Divertor Physics Design Studies"

7-9 November 1994, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Advisory Group Meeting on "Atomic, Molecular and Particle-Surface Interaction Data for Divertor Physics Design Studies"

7-9 November 1994, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Monday, November 7

09:30 - 10:00 Opening Address **Meeting Room: C07-V**
Adoption of Agenda

Session 1: Modelling of edge/divertor and similar low-temperature plasmas

Chairman: F. Brouillard

10:00 - 10:45: Reiter: Present A+M and PSI content of divertor modelling codes: new data needs for ITER divertor modelling

10:45 - 11:30: Bacal: Atomic and surface processes in H^- sources: relevance for divertor plasmas

11:30 - 11:45: Coffee Break

11:45 - 12:30: Capitelli: Vibrational population of molecular hydrogen in low-temperature plasmas

12:30 - 14:00: Lunch

Session 2: Electron-impact processes

Chairman: H. Tawara

14:00 - 14:45: Wadehra: Scattering of low-energy electrons from atomic and molecular hydrogen

14:45 - 15:30: Mitchell: Electron-molecular ion recombination and excitation processes

15:30 - 16:00: Coffee Break

16:00 - 16:30: Fujimoto: Towards a CR model for molecular hydrogen

16:30 - 17:00: Celiberto: Electron-impact processes of vibrationally excited hydrogen molecules

17:00 - 17:30: Fujimoto: Recent developments in the CR model for helium

17:30 - 18:00: Kato: Electron-impact excitation cross sections of carbon atoms and the line emission using the CR model

Tuesday, November 8

Session 3: Heavy particle collision processes

Chairman: J.B.A. Mitchell

09:00 - 09:45: Schultz: Elastic, momentum transfer and related cross sections for edge plasma relevant ion-neutral systems

09:45 - 10:30: Brouillard: Low-energy charge exchange processes in divertor plasmas

10:30 - 11:00: Coffee Break

11:00 - 11:30: Janev: Particle interchange reactions in hydrogen and hydrogen-helium collision systems

11:30 - 12:00: Tawara: Collision data of heavy particles involving excited species at low energies

12:00 - 12:30: Abramov: Some remarks about the low-energy charge exchange processes needed for ITER divertor modeling

12:30 - 14:00: Lunch

Session 4: Particle-surface collisions

Chairman: M. Bacal

14:00 - 14:45: Snowdon: Low-energy (1-100 eV) molecule-surface interactions

14:45 - 15:30: Heeren: Negative ion formation at surfaces

15:30 - 16:00: Coffee Break

16:00 - 16:45: Thomas: Status of particle reflection, electron ejection and sputtering databases

16:45 - 18:00: **Discussion:** What particle-surface interaction processes are the most important for the edge plasma physics, and what types of data are appropriate for the edge plasma modelling codes.

Wednesday, November 9

Session 5: Presence and role of vibrationally excited hydrogen molecules, H^- and H_3^+ in the plasma edge

Moderator: M. Capitelli

09:30 - 10:30: **Discussion:** (All participants)

- Participants should try to reach conclusions about the vibrational distributions of $H_2(v)$ and $H_2^+(v)$ in ITER divertor type plasmas and on the role of vibrationally excited species on the overall plasma and neutral gas kinetics and properties;
- Description of vibrationally excited species in the modelling codes.

10:30 - 11:00: Coffee Break

11:00 - 12:00: **Discussion:** (All participants)

Clarification of the following issues:

- Presence and life-time of H^- and H_3^+ ions in ITER divertor type plasmas and their role in plasma/neutral gas kinetics;
- Comments on three-body recombination processes in ITER divertor plasmas and status of their database.

12:00 - 14:00: Lunch

Session 6: Scope of the planned IAEA CRP on A+M and PSI data for fusion reactor divertor modelling and optimization

Chairman: R.K. Janev

14:00 - 15:30:
- Definition of the CRP scope;
- Suggestions for potential participants.

15:30 - 16:00: Coffee Break

16:00 - 17:00:
- Formulation and adoption of meeting conclusions and recommendations

Adjourn of the Meeting