



IAEA

International Atomic Energy Agency

INDC(NDS)- 0515
Distr. LP,NE,SK

INDC International Nuclear Data Committee

Atomic and Molecular Data for Plasma Modelling

Summary Report of Second IAEA Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

18 – 20 June 2007

Prepared by

Denis Humbert

November 2007

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/indc_sel.html or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to services@iaeaand.iaea.org
or to:

Nuclear Data Section
International Atomic Energy Agency
PO Box 100
Wagramer Strasse 5
A-1400 Vienna
Austria

Printed by the IAEA in Austria

November 2007

Atomic and Molecular Data for Plasma Modelling

Summary Report of Second IAEA Research Coordination Meeting

Prepared by

Denis Humbert

Abstract

A description is given of the proceedings, conclusions and recommendations of the second Research Coordination Meeting on “Atom and molecular data for plasma modelling”, held on 18-20 June 2007, at IAEA Headquarters in Vienna. During the course of the meeting progress achieved to date was thoroughly reviewed and many areas in need of further research were identified. Strong collaborations built during the course of this work have the potential to address these new issues. Therefore, one outcome of the RCM is a detailed proposal to extend the studies for two additional years with a final RCM early in 2009. Summaries are also given of the presentations made by the participants, along with the specific goals agreed for this Coordinated Research Project (CRP).

November 2007

TABLE OF CONTENTS

INTRODUCTION.....	7
OVERVIEW.....	7
PRESENTATIONS OF WORK PERFORMED.....	7
RESULTS ACHIEVED TO DATE AND FUTURE WORK PLAN.....	12
RECOMMENDATIONS AND CONCLUSIONS.....	16
APPENDICES	
APPENDIX 1: LIST OF PARTICIPANTS.....	17
APPENDIX 2: MEETING AGENDA.....	19

Introduction

The second Research Coordination Meeting (RCM) of the IAEA Co-ordinated Research Project (CRP) on “Atom and molecular data for plasma modelling” was held on 18-20 June 2007 at the IAEA Headquarters in Vienna. This meeting was saddened by news that John Hogan, representative of ORNL, passed away in November 2006. Dave Schultz, the new ORNL representative, presented a dedication to his memory. CRP participants will miss his high level of competence in plasma modelling and his cheerful personality.

The objectives of the meeting were as follows:

1. review the progress made on the work plan,
2. assess the activities undertaken towards achieving the specific objectives of the CRP.

All 14 CRP participants attended the meeting: Z. Herman (Czech Republic), K. Hassouni (France), U. Fantz (Germany), D. Reiter (Germany), M. Capitelli (Italy), M. Kimura, H. Tanaka (Japan), S. Matejcik (Slovak Republic), M. Larsson (Sweden), J. Tennyson (United Kingdom), B. J. Braams (USA), D. Schultz (USA), B. McLaughlin (United Kingdom, CRP observer) and R. K. Janev (Macedonia, consultant). The Agency was represented by A. L. Nichols, R. E. H. Clark and D. Humbert. The list of participants is attached as Appendix 1.

Overview

Attendees at the meeting were welcomed by A. Nichols (Head, Nuclear Data Section). He commented on the strong support of the Agency, the Division and the Section to fusion activities. The need for high quality data for the long-term success of the ITER project was noted.

Following the introduction, the proposed Agenda was reviewed and adopted without change (Appendix 2). The first two days were devoted to reports from the participants of their latest research activities related to the CRP, each participant giving forty-five min. talks including questions. Brief summaries of the presentations are reported below, while full presentations are available on the Web site of the A+M Data Unit (<http://www-amdis.iaea.org>). Much discussion resulted from the presentations, and areas meriting further research were noted. Detailed debate took place throughout late Tuesday afternoon and all Wednesday, including detailed discussions resulting from the presentations and areas with need for further research. A new work plan was defined with specific tasks agreed between the participants, and a request for an extension of the CRP was also formulated.

Presentations of Work Performed

During the course of the first two days, each participant summarised the results achieved to date. Participants gave a forty-five min. presentations, including questions - much discussion resulted and areas with need for further research were noted.

Z. Herman: Interaction of slow ions with surfaces; collisions of small hydrocarbon ions with carbon, tungsten and beryllium surfaces

Continuing his previous work on collisions of slow (15 – 45 eV) hydrocarbon ions with room-temperature and heated carbon surfaces, collisions of very slow (3 – 10 eV) hydrocarbon ions CD_n^+ ($n = 3, 4, 5$) with room-temperature carbon (HOPG) surfaces were investigated. The ion-surface scattering method is employed in which mass spectra, angular and translational energy distributions of ion products are determined. Survival probabilities of the projectile ions decreases below 10 eV to zero, from about 10% for CD_5^+ and about 0.3% for CD_3^+ and CD_4^+ (incident angle 30°). Kinematic

analysis of the data helps to elucidate the collisional mechanisms and the effective mass of the surface for collision of the very slow ions.

Collisions of selected slow (15 – 45 eV) hydrocarbon ions (CD_5^+ , CD_4^+ ; $C_2D_4^+$, $C_2D_5^+$) with room-temperature and heated tungsten and beryllium surfaces show that the survival probability of the projectile ions is usually 5 to 10 times smaller than on carbon surfaces. However, impurities on freshly prepared surfaces lead to deflections of up to 5% of the incident ions away from the surface without collision due to surface charges. The results of inelastic collisions with heated and room-temperature W-surfaces are rather similar to those with the carbon surfaces (extent of fragmentation, chemical reactions, angular distributions and energy losses). Resulting structures on beryllium surfaces identified with angular and translational energy distributions indicate several different processes that are presumably connected with scattering from different materials on the surface (oxides, carbides and hydrocarbon layers).

M. Larsson: Progress in measurements of dissociative recombination

Mats Larsson described how an ion storage ring can be used to measure product branching ratios in dissociative recombination of molecular ions. Results for hydrocarbon ion recombination obtained at the storage ring CRYRING were summarized.

The long and controversial debate about the dissociative recombination of H_3^+ was reviewed, and new experimental and theoretical results were presented. A database for the dissociative recombination of molecular ions was also described.

S. Matejcik: Electron Impact Ionization (EII) of plasma edge constituents; properties of Be_xH_y molecules

Small hydrocarbon molecules and their isotopomer are formed in the edge plasma of fusion reactors. The kinetic and thermochemical data quantifying electron impact ionization of these molecules are of high relevance to the fusion edge plasma - Matejcik presented work he has undertaken on their electron impact ionization. Appearance energies for several molecules (CH_4 , CD_4 , CH_3D , C_2H_6 , ...) have been measured at two different temperatures (300 and 700K), and thermal and isotopic effects have been observed. Recently, measurements have been made of the appearance energies of the C_2D_6 molecule and the partial cross section for electron impact ionization into several fragment ions. Future plans include cross-section measurements to form other hydrocarbon molecules.

Several new materials are being considered in the design of fusion reactors, and beryllium is one of the candidates for the blanket. Studies of the properties of small molecules and clusters formed from beryllium using advanced quantum chemical methods (CSSD(T)-R12, CSSD(T)-full, MP2, B3LYP) were reviewed. Matejcik presented results on the calculation of the structures and the dissociation energies of BeH and BeH_2 molecules, including the excited states of these molecules. Structure and atomisation energy have been studied for the beryllium hydrides: Be_nH_m ($n=1 \leq n \leq 4$, $1 \leq m \leq n$) clusters.

B.J. Braams: Reaction dynamics and spectroscopy of hydrocarbons in plasmas

The work presented by Braams is part of a project with Joel Bowman (Emory University), Ralf Schneider and Amit Sharma (IPP Greifswald) to construct potential energy surfaces and carry out molecular dynamics studies and spectroscopic modelling of molecules and reaction complexes $C_2H_m^+$ and $C_3H_m^+$ ($m \leq 5$) in plasmas. The initial studies involved $C_2H_3^+$ [1], and work is now underway on $C_2H_5^+$. Braams reviewed the different tools for the construction of potential energy surfaces, described the MULTIMODE analysis of the ro-vibrational spectrum and quasi-classical trajectory calculations for reaction dynamics, including plans for the next two years. A principal challenge will be to handle non-adiabatic effects (surface crossings) in the reaction dynamics, which is essential in the modelling of charge exchange reactions.

[1] Amit R. Sharma *et al.*, Potential energy surface and MULTIMODE vibrational analysis of $C_2H_3^+$, *J. Chem. Phys.* **125** (2006) #224306.

M. Capitelli: Elementary processes, transport and kinetics of molecular plasmas

Capitelli presented the relevant results obtained by his research group, reporting first on the elementary processes and then on the transport properties of H_2 plasmas.

Elementary processes:

- Proceeding through the low-lying Rydberg states ($B^1\Sigma_u^+$, $D^1\Pi_u$), state-to-state radiative decay-vibrational excitation cross sections for EV processes, have been calculated for H_2 and D_2 molecules. The alternative exit channel (i.e. decay to the continuum of the ground state resulting in the molecular dissociation (*radiative decay dissociation*)) has also been considered, deriving corresponding state-resolved cross sections.
- Proceeding through the $^2\Sigma_g^+$ excited state of H_2^- molecular ion (*14 eV resonance*), resonant vibrational excitation cross sections in eV processes have been obtained by using the local resonance model with resolution on the final vibrational level, showing good agreement with experiments.
- Resonant charge transfer processes have been studied in collisions involving atom-parent ion, both in electronically excited states for nitrogen systems, using the asymptotic approach.
- Cross-sections and rate coefficients for atom-molecule system involving hydrogen isotopes have been calculated by the quasi-classical trajectory method, with resolution on the roto-vibrational level of the molecular target using a new and more accurate potential energy surface. Moreover, scaling relations that allow the derivation of accurate cross-sections for different colliding systems from the QCT hydrogen complete database have been verified.
- Nitrogen atom-molecule processes – quasi-classical calculations have been extended in translational energy up to 9 eV (previous limit was 3eV). This allows a more reliable calculation of rate coefficients for temperature ranges extending to 10000K and over. For the purpose of practical usage in kinetic codes, complete analytical fittings of rate coefficients for both vibrational energy exchange and state specific dissociation have been performed.
- Harpoon reactions involving caesium and hydrogen molecules in highly excited electronic states have been studied in terms of the asymptotic approach for resonant processes.

Transport cross-sections of electronically excited states of atomic hydrogen have been derived by using semiclassical approaches, and used to calculate the transport coefficients (viscosity, thermal conductivity and electrical conductivity) of thermal plasmas in a wide range of temperatures and pressures, including the effect of external magnetic fields. A tensorial reformulation of the Chapman Eskog theory was required along with the implementation of a new numerical code. The results show the strong influence of excited states on transport.

U. Fantz: Compilation, calculation and validation of fundamental data for diatomic molecules

The compilation of atomic and molecular data for plasma edge modelling is focussed on atomic and molecular hydrogen (and isotopomers) and on hydrocarbon species, i.e. CH and C_2 molecules. Franck-Condon factors and transition probabilities are calculated with the *TraDiMo* code on the basis of potential curves and dipole transition moments compiled from the literature. The available data set for transitions in hydrogen molecules has been extended by calculating transitions from the hydrogen molecule to the ground state of the molecular hydrogen ion. Vibrationally resolved cross-sections and

rate coefficients for electron impact collisions are compiled from the literature and, if not available, calculated using the *IPProg* code which is based on the Impact Parameter method. Data sets for CH and C₂ were presented, which are also the basis for collisional radiative modelling using the flexible *Yacora* code. The analysis of populating and depopulating processes allows for an assessment of their relevance in the plasma edge, e.g. calculations of photon emissivity coefficients. Heavy particle collisions in the modelling of the dissociation of hydrocarbons were addressed by means of *Yacora* calculations. Calculated population densities and particle densities can be validated by performing dedicated laboratory and plasma edge experiments.

R. Janev: New collision data for H/H₂ and C_xH_y databases

Janev reported on new cross-section results for the following processes:

1. resonant vibrational excitation and dissociative attachment in e-H₂ collisions over the energy range from 11 to 14 eV;
2. mutual neutralization in slow collisions of H⁻ with H₂⁺ and H₃⁺ ions;
3. electron impact excitation of X → A and X → B transitions in CH;
4. dissociative excitation and ionization of CD_y⁺ ions by electron impact.

The results for processes (1) – (3) were obtained from theoretical calculations (those for (3) in collaboration with Profs. R. Celiberto and J.Wadehra), while those for processes (4) were extracted by analysis of the total DE +DI experimental cross sections of the Louvain-la-Neuve group (Prof. P. Defrance) in collaboration with members of that group.

H. Tanaka: Electron collision data of C-H and C-F compound molecules for plasma modelling

Tanaka reported on the present status of different databases compilations. Compilations are available in various reports – *Elastic Differential Cross sections for Electron Collisions with Polyatomic Molecules*, and *Database for Electron Collisions with Polyatomic Molecules: Elastic- and Resonant Vibrational Excitation-Differential Cross Sections*. Experimental results were also presented on electron-polyatomic molecules for the neutral radical formation from CH₄ as well as for the spectroscopy of molecules related to the plasma modelling.

M. Kimura: Charge transfer cross sections in H⁺, He²⁺, C⁺-molecule collisions; surface absorbed atom/molecule case

Kimura reported on charge transfer cross-sections that were systematically determined by joint experimental and theoretical investigations for H⁺, He²⁺ and C⁺ ion impacts on various molecular targets in collision energy from a few tens of eV to 25 keV/u. Target molecules were primarily selected from hydrocarbons (C_nF_m, n < 4), but were also extended to include H₂, H₂O, CO, CO₂ and O₂ molecules. For most cases, there have been no other investigations, and these results are the very first to be obtained. For collisions of He²⁺ ion on H₂ molecules, the present double-charge transfer cross-sections are found to differ significantly from earlier data which show an increase as the collision energy decreases. Hence, even for these most basic collisions systems, uncertainties in the cross-sections and dynamics still remain. Kimura and his research group have also investigated charge transfer from H and Na atoms absorbed on Al surface. The collision dynamics and corresponding cross-sections from surface absorbed atoms are found to be quite different from those in the gas phase.

B. McLaughlin: Electron collisions with small molecular hydrides

Low energy electron collisions with small molecular hydrides are being investigated for a number of different complexes using the R-matrix method. McLaughlin presented the current status of such calculations for molecules relevant to plasma modelling. Elastic and inelastic cross-sections for systems such as BeH, BeH₂, CH and CH₂ were addressed.

J. Tennyson: Calculated molecular data for fusion plasmas

Tennyson presented various results obtained using the R-Matrix method and the recently developed Molecular R-Matrix with Pseudo-State (MRMPS). The R-matrix method provides a rather general procedure for treating electron molecule collisions at low energies based on close-coupling expansion, representing a powerful *ab initio* means of providing curves and widths for studies of dissociative recombination of small molecular cations such as NO^+ . A recent application of this procedure is the bound and continuum of potential energy curves for CO^+ .

An altogether more challenging problem is the study of resonances in molecular anions such as C_2^- because the resonance structure in C_2^- lies above the electron detachment threshold. Under these circumstances, the close-coupling expansion fails. The MRMPS method in principle can solve this problem, but becomes computationally very expensive for many-electron problems. However, combining MRMPS calculations with the partitioned R-matrix procedure has allowed stable scattering calculations to be performed to address this problem for the first time.

K. Hassouni: Modeling dust formation in carbon-containing discharge plasmas

Hassouni presented specific aspects of the modelling of H_2 , H_2/CH_4 , $\text{Ar}/\text{H}_2/\text{CH}_4$, soot and poly aromatic hydrocarbons (PAH) formation in microwave plasmas. A significant emphasis was placed on the problems related to collisional data. The first part of the presentation dealt with the modelling of the kinetics and the development of a collisional radiative model for a pure H_2 plasma. Effects of the vibrationally and electronically excited states on the overall dissociation and ionization kinetics were also studied. Major data needs apply to near-threshold cross-sections for intermediate (8 – 20 eV) threshold processes.

The H_2 model can be reduced to obtain simple and accurate chemical models that may be used in transport codes and in the modelling of the more complex H_2/CH_4 and $\text{Ar}/\text{H}_2/\text{CH}_4$ plasmas. The 2C Model considers only two hydrocarbon species, and is in good agreement with experimental data. Both the A4 and A9 Models deal with the mechanism of PAHs and soot formation - results show significant particle nucleation at low temperatures (< 1500K). There remains a strong need for data to validate these models.

Finally, experimental results and modelling of carbon nucleation growth and transport of dust in DC discharges ignited in argon plasma were presented.

D. Reiter: Atomic and molecular data issues for ITER, and status of databases for the EIRENE code

After briefly recalling the ITER divertor concepts and the expected plasma conditions in this domain with particularly intense plasma-surface interaction, Reiter explained the critical design issue of tritium retention in magnetic fusion devices. JET had been operated with a D-T mixture, and a build-up of tritium in the machine was observed without any sign of saturation. Also the location of the resulting tritium was surprising: most tritium was recovered in quite remote areas with no direct plasma contact. Radiation safety considerations for ITER lead to a maximum tolerable level of approximately 500 mg of mobile tritium in the machine (this limit being defined by air leakage, water leakage and other off normal events). Extrapolation of plasma-surface fluxes and surface erosion in the form of chemical sputtering (formation of hydrocarbons) results in very pessimistic estimates for ITER with respect to availability of the machine. This issue needs to be better quantified and understood. Therefore, the atomic and molecular data package of the *EIRENE* code (e.g. used by the ITER team for divertor design studies) has been upgraded by an extensive set of hydrocarbon collision cross-sections over a wide energy range. This database is continuously being updated with new results from the present IAEA CRP - available online under: www.hydkin.de

Along with the full set of cross-sections, integration into rate coefficients has been provided online, as well as solution of a set of time-dependent, 0-dimensional rate equations for hydrocarbon catabolism

in hydrogen-electron plasmas. This online solver also provides a time-scale analysis (for separation of fast vs. slow chemical timescales in the system), as well as an analytical sensitivity analysis of the results on any of the rate constants in closed form.

Implementation of surface data (reflection and re-emission of hydrocarbons) into this system of rate equations is ongoing, which is based on molecular dynamics calculations (Ruzic, University of Illinois, USA; Sharma and Schneider, MPI Greifswald, Germany).

D.R. Schultz: Overview of the capabilities of the ORNL Atomic Physics Group

A brief overview of the fusion energy relevant portion of the atomic physics program at Oak Ridge National Laboratory (ORNL) was presented by Schultz, who has replaced the late J.T. Hogan within the CRP. The three components of the program were described, namely the Controlled Fusion Atomic Data Center, the Multicharged Ion Research Facility, and the theoretical and computational physics activities. Consideration was also given to the capabilities that could be called upon for data production within the context of the present CRP. The most likely synergies were in the area of inelastic electron-impact processes involving hydrocarbons: new experiments will be encouraged to test and extend the existing data in this area. Robust experimental and theoretical efforts at ORNL in the study of particle-surface interactions were also noted. However, these capabilities were judged to be more closely aligned with the scope of work for another CRP that is about to begin.

Results Achieved To Date and Future Work Plan

During the Tuesday afternoon session chaired by Capitelli and the Wednesday morning session chaired by Reiter, the work plan was thoroughly reviewed; Tennyson undertook the task of rapporteur. Specific areas were identified with the need for further investigation.

CRP participants have focused on gathering and generating new data relevant to modelling the edge region of plasmas within nuclear fusion energy devices. The work plan is divided into two topics: plasma surface interactions, and volume processes. Each participant presented the work achieved from the work plan formulated during the first RCM (given below *in italics*), and defined those tasks remaining to be done. Every participant commented on and suggested changes and extensions to the work to be done as the discussions unfolded.

Surface processes

Include low-energy D and chemical reactions for $C \rightarrow C_3$ hydrocarbons at energies from 1 to 10 eV (consider neutrals as well as ions) and evaluate present database. Also investigate other surfaces: Be and W, and compare ion survival from C/Be/W [Herman].

Achieved: $C_nD_m^+$ ($n = 1, 2, 3$) hydrocarbons - ion survival probability, energy transfer to solid, fragmentation and chemical reactions at surface, as well as collision kinematics were studied with the following conditions and surfaces:

- at room-temperature and 600° over the incident energy range 15 - 50 eV for collisions on C, Be and W surfaces
- at room-temperature over the incident energy range 2-10 eV for C surface.

Tasks: extend measurements for Be and W surfaces to 2 to 10 eV; also study chemically modified surfaces.

Evaluate the Alman/Ruzic/Brooks surface database in fusion plasma modelling “A hydrocarbon reaction model for low temperature hydrogen plasmas and an application to the Joint European Torus”, D. Alman, D. Ruzic, J. Brooks, Physics of Plasmas 7 (2000) 1421 [Schultz, Reiter].

Achieved: evaluation is still open. Most data are available from Sharma *et al.* with some gaps in energy range and species coverage.

Task: complete and edit database. Schultz will supply electronic version of data and will provide link data providers. Undertake a sensitivity analysis; data validation remains an issue.

Determine experimental signatures of surface productions of molecules such as C₂H₂ and other ITER relevant molecules, as well as diamond-like carbon (DLC). Mass spectrometry. Evaluate present database [Hassouni].

Achieved: experimental set up has been established. Experiments were carried out at low temperature (up to 500°C).

Task: Study higher temperature to achieve chemical erosion with H.

Most basic hydride - study recombination of atomic H/D onto graphite to understand formation of vibrational excited molecules [Capitelli].

Achieved: everything

Task: study H and H₂ on W and Fe surfaces.
define relationships with other CRPs.

Volume processes

Scheme:

QC → scattering theory/experiment → experimental validation (spectroscopy, fusion experiments) → relevant fusion applications (ITER)

Calculate ground state potential energy surfaces for hydrocarbons to C₂H₆ [Braams].

Achieved: work in progress. Data have been calculated for all species. Some surfaces are complete.

Task: C₃ and C₄ species will be included. Charged species will be considered.

Evaluate cross-section reaction rates (vibrational and rotationally-resolved) for reactions proceeding on the ground state surface; evaluate the relevance of ground state restriction to edge plasma processes. Provide ionization potentials, thresholds, ro-vibrational cross sections and spectroscopic data for reactions [Braams].

Achieved: work in progress

Task: [H-hydrocarbon]⁺ processes will be considered.

Complete database of e-collision cross sections for vibrational excited molecules (D₂, DT, T₂), and continue work on atom-diatom, electron-molecule collisions [Capitelli].

Achieved: electron-H₂ isotopologues database is complete for vibrationally resolved transitions from X state to singlet excited states. Also included some triplet-triplet transitions with n < 4.

Task: complete work for all isotopologues and realize a benchmark comparison with R-matrix results at lower energies.

For the atom-molecule collisions, compare the results with the data from Krstic *et al.* for H-H₂ and H⁺-H₂ collisions.

Calculate electronic structure, binding energy, volatility affinities and ionization energies for Be_{1,2}, hydrides and H₂ reactions with Be_n clusters [Matejcik].

Achieved: structure and energetics calculations completed for small Be hydrides and Be clusters including some excited states.

Task: compute ionization energies and further excited states. Identify negative ion resonances.

Calculate excited state molecular structure up to C₄H₈.

Evaluate CO sticking on metallic substrate surfaces (Ag) [Kimura].

Achieved: completed electronic structure calculations on hydrocarbons.

Task: nuclear motion calculations – identification of fragmentation pathways on excited states. CO sticking and desorption calculations.

Determine charge-transfer cross-sections in collisions of H^+ , He^{2+} and C^{q+} ions with hydrocarbons and other fusion-relevant molecules systematically below 50 keV/u [Kimura].

Achieved: completed calculations on C^+ at higher energies.

Task: extend calculations to lower collision energies.

Determine fragmented species from impurity molecules after charge transfer and ionization, and their energy distributions [Kimura].

Achieved: CH_4 and C_2H_2 .

Task: extend to higher hydrocarbons.

Evaluate theoretical cross sections (R-matrix) on total, elastic and inelastic electronic excitation (energy 1-10 eV) of the diatomic molecules BeH, BeD, CD and C_2 . Then extend to the polyatomic systems, BeH_y , and isotopomers, and hydrocarbon molecules (CH , C_2H_2 and C_2) [Tennyson, McLaughlin].

Achieved:

initial studies for (elastic and inelastic) electron collisions on BeH, BeH_2 , CH, CD and CH_2 have been performed [McLaughlin].

Elastic and inelastic collisions with C_2 ; elastic electron collisions with HCCH were performed [Tennyson].

Tasks:

complete above studies and include vibrational effects correctly.

Extend range (energy and geometry) of electron H_2 studies [Tennyson].

Consider CH^+ .

Evaluate electron-C atom collisions (elastic and momentum transfer cross sections)? [McLaughlin]

Benchmark C_2H_2 rates, electron collision cross-sections.

Elastic, vibrational and electronic excitation (break-up) [Tennyson, McLaughlin, Tanaka].

Achieved: experimental elastic and vibrational excitation cross-sections are available. Calculated elastic cross-sections are complete.

Task: perform theory and experiment for electronically inelastic cross-sections.

Ionization data for C_2H_2 [Braams, used as input by Hassouni].

Achieved: ionization threshold for C_3H has been performed.

Query: Investigate effect of vibrational distribution in plasma on processes such as near threshold ionization of HCCH?

Closed shell hydrocarbon molecules:

1) provide missing but necessary experimental data – cross-sections for the excited neutral molecular species and the emissive radical production from C-H compound molecules by low-energy electron impact;

2) unification of database for modelling at Jülich, and updating of the database [Tanaka et al].

Achieved:

1) **EELS:** provided the DCS of C-H and C-F compounds of C_3H_6 isomers, CF_3X ($X = Cl, Br$), and 1,1- $C_2F_2H_2$, C_6H_5X ($X = H, CH_3, CF_3$), H_2 , CO, NO by electron impact,

2) **QMS:** determined the cross-section for the neutral non-emissive radical of CH_3 production from CH_4 by electron impact in the threshold region and observed the negative ion formations, CH_3^- , CH_2^- , CH^- , C^- that originated either from gas or surface phase,

3) **Database:** compiled the data on *Elastic DCS for Electron Collisions with Polyatomic Molecules*

Tasks:

1) **EELS:** continuous and systematic provision of the DCS of plasma-relevant C-H and C-F compounds by electron impact; and, as the targets for electron collision, employs the vibrationally excited molecule (hot molecule produced in our SR experiment) to study the temperature effect on the cross-section as well as the clean W, Be, and C surfaces to determine the ratios of elastic and inelastic scattering of electron from those surfaces,

- 2) **QMS**: measures the neutral non-emissive radicals of $\text{CH}_{2,1}$ and negative ion formations from CH_4 by electron impact in the threshold region,
- 3) **Database**: revision of the IAEA and NIFS report *Database for Electron Collisions with Polyatomic Molecules: Elastic-, Resonant Vibrational-, and Electronic Excitations* – to provide differential cross sections as both IAEA and Julich database(?) (including the Yong-ki Kim scaling law).

Merged and completed databases to be available both from FZ-J and IAEA NDS A+M Unit [Reiter, Janev, Clark].

Status: ongoing. All results are available on the Jülich web site: www.hydkin.de

Task: create documentation. Extend the database to H data.

C_3H_x ionic systems - recombination, and dissociation excitation.

Cross-sections as well as rates. Evaluate relevance of BeH^+ , BeH_2^+ [Larsson].

Achieved: measurements and calculations for C_3H_x , $x = 4$ and 7 as well as C_4D_2 and D_2H^+ . Measurements on Be have not been undertaken because CRYRING is unable to handle such a system.

Task: Perform calculations on BeH^+ . DR on CH_4^+ .

Coordinate with the above task. Explore effect of target temperature? [Schultz]

Measure ionization – cross-sections in threshold region to 10 eV, for CH_4 , C_2H_6 , C_3H_8 and fragments. Propane cross-section at elevated T of 700K [Matejcik, Hassouni].

Achieved: measurement of C_3H_8 and C_2D_6 at low temperature.

Task: extend energy range up to 150 eV and complete other projects. Cover a range of temperatures.

CR modelling, data from Bari for H_2 (D_2). Differences in excitation for isotopes? Validate for HD in ECR discharges. [Fantz]

Achieved: tools are available for H_2 .

Task: Need input data to complete modelling. Perform scaling test.

CR modelling for C_2/CH molecules - FC factors, systematic transition probabilities, and eventually BeH/BH for diagnostic applications. [Fantz]

Achieved: simplified version for C_2/CH .

Task: C_2/CH - check number of electronic levels sufficient; improve data.

Check approximation for CH using R-matrix data from McLaughlin.

BeH data from Matejcik; collisional data from McLaughlin.

BH lower priority.

CR/dissociation modelling to determine PECs for CH, C_2 , H_2 to test available databases, and generate information about recombination processes. ECR plasmas + AUG/DIII-D comparisons.

See how heavy-particle collisions influence dissociation modelling, and determine relevance to divertor plasmas [Fantz].

Achieved: measurements have been performed. Models do not reproduce all observations.

Task: improve database and model. Test sensitivity to inclusion of chemistry.

Extend model used previously to study DLC to lower pressure (few Pa) with PIC for C_2H_2 and CH_4 to deduce main species, plasma and surface chemistry from experiments - e-impact vs CX [Hassouni].

Achieved: experiments are running with pure H and graphite target.

Task: provoke erosion of graphite by heating.

Apply CR model to H_2 -H system in order to evaluate the validity of this approach through collaboration with Augsburg/AUG [Hassouni, Fantz, Capitelli].

Achieved: CR model was successfully applied to Augsburg experiment (AUG and negative ion sources). Problems with CR model were identified; some of these difficulties have been fixed.

Task: continue comparisons.

Supply data on H_2 excited state processes. [Janev]

Line shapes (CH, C₂, C) to give information on kinetics of break-up [Fantz].

Achieved: laboratory measurements show two rotational temperatures due to break up dynamics. Further investigations have low priority.

Integrated modelling for tokamaks, stellarators and ITER. Evaluation of the impact of new data on plasma observables, especially through spectroscopy. Assess and report differences in database predictions for hydrocarbon break-up chain-integrated models (for example, J-R vs E-L, A-R). Direct application to JET and ITER divertor modelling. Assess sensitivity to break-up kinetic energies, and evaluate effects on line shapes (CH, C₂, C) [Hogan, Reiter].

Achieved: extended to C ions. Studies of break-up kinetics have been performed. J-R/E-L databases have been compared.

Task: more cross sections are required for the CR model for atomic C.

Application to JET and ITER ongoing.

Data on fragmentation of hydrocarbons at surfaces. [Janev]

The detailed list of outcomes and further tasks to be performed reveals a number of areas that merit further investigation with respect to both surface and volume processes:

Data needs for surface processes: the CRP does not have enough expertise to address these issues within the agreed duration of the project. These areas should be addressed during the course of the next two scheduled CRPs on “surfaces erosion” and “formation of dust in tokomaks reactors” - close collaboration between these CRPs is also highly recommended.

Volume processes: work achieved and the proposed detailed work plan show that the CRP would benefit greatly from an extension of two years. Therefore, a detailed proposal for a two year extension has been formulated, with a final RCM in early 2009.

Recommendations and Conclusions

The CRP on “Atomic and molecular data for plasma modelling” has focused on the gathering and generation of new data relevant to the edge region of plasmas in nuclear fusion energy devices. Presentations and discussions showed that this CRP has been very successful in producing new data essential for the modelling of the plasma edge region with respect to surface and volume processes. A number of areas have been identified that will greatly benefit from an extension of the CRP by a further two years. Work achieved during the first 1.5 years of the CRP was described in detail, and new tasks were agreed by and assigned to the participants. A detailed proposal for a two-year extension was formulated that includes a final RCM in early 2009 - this extension will take advantage of the existing collaborations among the existing participants. New data produced by this CRP are in the process of being prepared for inclusion in ALADDIN, the IAEA AM/PSI numerical database.

IAEA 2nd Research Coordination Meeting: Atomic and Molecular Data for Plasma Modelling

18–20 June 2007, building-A, floor-04, room-78 (A04-78), IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis HumbertLIST OF PARTICIPANTS

Dr. Zdenek Herman
 V. Cermak Laboratory
 J. Heyrovsky Institute of Physical Chemistry
 Academy of Sciences of the Czech Republic
 Dolejskova 3
 CZ-18223 Praha 8
 CZECH REPUBLIC
 Tel.: +420-2-66053514; Fax: +420-2-8582307
 E-mail: zdenek.herman@jh-inst.cas.cz

Prof. Khaled Hassouni
 Laboratoire d'Ingénierie des Matériaux et des
 Hautes Pressions
 Université Paris XIII
 Av. J. B. Clément
 F-93430 Villetaneuse
 Tel.: +33-1-4940-3411; Fax: +33-1-4940-3414
 E-mail: hassouni@limhp.univ-paris13.fr

Dr. Ursel Fantz
 Lehrstuhl für Experimentelle Plasmaphysik
 Institut für Physik, Universitätsstr. 1
 D-86135 Augsburg
 GERMANY
 Tel.: +49-821-598-3310; Fax: +49-821-598-3302
 E-mail: fantz@physik.uni-augsburg.de

Prof. Dr. Detlev Reiter
 Forschungszentrum Jülich GmbH
 Institut für Plasmaphysik (IPP)
 D-52425 Jülich
 GERMANY
 Tel.: +49-2461-61-5841; Fax: +49-2461-61-2970
 E-mail: d.reiter@fz-juelich.de; d.reiter@eirene.de

Prof. M. Capitelli
 Centro di Studio per la Chimica de Plasm
 Dipartimento di Chimica
 Università di Bari
 Via Orabona 4
 I-70126 Bari
 ITALY
 Tel.: +39-80-544-2104; Fax: +39-80-544-2024
 E-mail: mario.capitelli@ba.imip.cnr.it

Prof. Mineo Kimura
 Department of Chemistry
 Faculty of Sciences
 Graduate School of Sciences
 Kyushu University
 6-10-1 Hakozaki, Higashi-ku
 Fukuoka 812-8581
 JAPAN
 Tel.: +81-92-642-2592; Fax: +81-92-642-2607
 E-mail: mineoscc@mbox.nc.kyushu-u.ac.jp

Prof. Hiroshi Tanaka
 Faculty of Sciences and Technology
 Sophia University
 7-1 Kioi-cho, Chiyoda-ku
 Tokyo 102-8554
 JAPAN
 Tel.: +81-3-3238-3472; Fax: +81-3-3228-3341
 E-mail: h_tanaka@sophia.ac.jp

Dr. Ratko K. Janev
 Macedonian Academy of Sciences and Arts
 Bulevar K. Misirkov, 2
 P.O. Box 428
 91000 Skopje
 MACEDONIA
 Tel.: +389-91-114200; Fax: +389-91-114685
 E-mail: rjanev@manu.edu.mk

Dr. Stefan Matejčík
 Dept. of Plasmaphysics
 Comenius University
 Mlynska dolina F2
 SK-84215 Bratislava
 SLOVAK REPUBLIC
 Tel.: +421-7-60295686; Fax: +421-7-65425882
 E-mail: matejčík@fmph.uniba.sk

Dr. Mats Larsson
 Department of Physics
 AlbanNova
 Stockholm University
 SE-106 91 Stockholm
 SWEDEN
 Tel.: +46-8-5537-8647; Fax: +46-733-894377
 E-mail: mats.larsson@physto.se

Dr. Brendan M. McLaughlin
Department of Applied Mathematics and
Theoretical Physics
The Queen's University of Belfast
Belfast, BT7 1NN
Northern Ireland
UNITED KINGDOM
Tel.: +44-28-90273369; Fax: +44-28-90239182
E-mail: b.mclaughlin@qub.ac.uk

Dr. D. Humbert
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21729
Fax: +43-1-26007
E-mail: d.humbert@iaea.org

Dr. Jonathan Tennyson
Department of Physics & Astronomy
University College London
Gower Street
London, WC1E 6BT
UNITED KINGDOM
Tel.: +44-20-7679-7809; Fax: +44-20-7679-7145
E-mail: j.tennyson@ucl.ac.uk

Dr. Bastiaan J. Braams
Visiting Associate Professor
Math and Computer Science Department
Emory University
E430 Math & Sciences Building
400 Dowman Drive
Atlanta, GA 30322
U.S.A.
Tel.: +1-404-727-1980; Fax: +1-404-727-5611
E-mail: braams@mathcs.emory.edu

Dr. David R. Schultz
Physics Division
Oak Ridge National Laboratory
MS 6372, Bldg. 6003
P.O. Box 2008
Oak Ridge, Tennessee 37831-6372
U.S.A.
Tel.: +1-865-576-9461; Fax: +1-865-576-1118
E-mail: schultzd@ornl.gov

I.A.E.A.

Dr. R.E.H. Clark
IAEA Atomic and Molecular Data Unit
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA
Tel.: +43-1-2600-21731
Fax: +43-1-26007
E-mail: r.e.h.clark@iaea.org

IAEA 2nd Research Coordination Meeting: Atomic and Molecular Data for Plasma Modelling

18–20 June 2007, building-A, floor-04, room-78 (A04-78), IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

MEETING AGENDA

Monday, 18 June

09:15 – 09:45 Opening, Adoption of Agenda, A. Nichols, R.E.H. Clark, D. Humbert

Session 1: Scientific Reports

Chairman: J. Tennyson

09:45 – 10:30 Z. Herman Interaction of slow ions with surfaces: collisions of small hydrocarbon ions with carbon, tungsten, and beryllium surfaces ([abstract](#))

10:30 – 11:00 *Coffee Break*

11:00 – 11:45 M. Larsson Progress in measurements of dissociative recombination

11:45 – 12:30 S. Matejcik EII of plasma edge constituents, properties of Be_xH_y molecules

12:30 – 14:00 *Lunch*

Session 2: Scientific Reports (Continued)

Chairman: H. Tanaka

14:00 – 14:45 B. Braams Studies of reaction dynamics and spectroscopy of hydrocarbons in plasma ([abstract](#))

14:45 – 15:30 M. Capitelli Elementary processes, transport and kinetics of molecular plasmas ([abstract](#))

15:30 – 16:00 *Coffee Break*

16:00 – 16:45 U. Fantz Compilation, calculation and validation of fundamental data for diatomic molecules ([abstract](#))

16:45 – 17:30 R. Janev New collision data for H/H₂ and C_xH_y databases ([abstract](#))

Tuesday, 19 June

Session 3: Scientific Reports (Continued)

Chairman: M. Larsson

09:00 – 09:45	H. Tanaka	Electron collision data of C-H and C-F compound molecules for plasma modeling (abstract)
09:45 – 10:30	K. Kimura	Charge transfer cross sections in H^+ , He^{2+} , C^+ -molecule collisions: surface absorbed atom/molecule case
10:30 – 11:00	<i>Coffee Break</i>	
11:00 – 11:45	B. McLaughlin	Electron collisions with small molecular hydrides (abstract)
11:45 – 12:30	J. Tennyson	Calculated molecular data for fusion plasmas
12:30 – 13:45	<i>Lunch</i>	

Session 4: Scientific Reports (Continued)

Chairman: B. Braams

13:45 – 14:30	K. Hassouni	Modeling dust formation in carbon-containing discharge plasmas: <i>major molecular data needs</i>
14:30 – 15:15	D. Reiter	Atomic and molecular data issues for ITER, and status of databases for the EIRENE code
15:15 – 15:45	<i>Coffee Break</i>	
15:45 – 16:30	D. Schultz	Brief overview of the ORNL Atomic Physics Group's capabilities

Session 5: Review of Work Plan and Outcomes

Chairman: M. Capitelli

16:30 – 17:15	All	Discussion
---------------	-----	------------

Wednesday, 20 June

Session 6: Formulation of Meeting Conclusions and Reports

Chairman: D. Reiter

09:00 – 10:45 All Discussion of reports and database additions

10:45 – 11:15 *Coffee Break*

11:15 – 12:30 All Formulation of meeting conclusions

12:30 – 14:00 *Lunch*

Session 6: Formulation of Meeting Conclusions (Continued)

Chairman: D. Schultz

14:00 – 16:00 All Discussion and possible formulation of proposal to extend this
CRP

16:00 – *Adjournment of Meeting*

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710
Web: <http://www-nds.iaea.org>
