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Atomic Data for Vapour Shielding in Fusion Devices

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria
13 – 15 March 2019

Prepared by
K. Heinola

May 2019

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Abstract

The First Research Coordination Meeting of the Coordinated Research Project on *Atomic Data for Vapour Shielding in Fusion Devices* was held at the IAEA Headquarters in Vienna on 13 – 15 March 2019. Nine experts representing nine research institutes globally (Australia, China, India, Italy, Netherlands, North Macedonia, Spain, Syria, USA) in the field of atomic collisional physics and vapour formation for magnetic confinement fusion devices met together with the IAEA staff. The participants were theorists and modellers of plasma and vapour particle collisional processes, experimentalists of spectral line properties, and vapour formation and spectral analyses. They described their research background, available experimental methodologies and theories applied in various computational tools. Open issues related to elemental particles formed during vapour evolution and the particle interaction processes were discussed and plans for coordinated research to be performed during the project were made. The proceedings of the meeting are summarized in this report.

May 2019

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Abbreviations

Computational

AOCC	Atomic Orbital Close Coupling
BPRM	Breit-Pauli R-Matrix calculations
CCC	Convergent Close-Coupling Theory
CIV3	atomic structure calculations using Configuration Interaction technique
CMD	Classical Molecular Dynamics simulations
CR	Collisional-Radiative model
CTMC	Classical Trajectory Monte Carlo calculations
DARC	Dirac Atomic R-Matrix code
DC-DFTB-K	Divide-and-Conquer Density Functional Tight Binding method for large systems
DFT	electron Density Functional Theory
EEM	Electronegativity Equalization Method
FAC	Flexible Atomic Code
GRASP2K	code for energy level and radiative rate calculations employing MCDHF
LAMMPS	code for CMD calculations
MCDHF	multiconfigurational Dirac-Hartree-Fock method
MOCC	Molecular Orbital Closed Coupling
MOLPRO	Package of codes for molecular electronic structure calculations
MRDCI	Multi-reference single- and double-excitation configuration interaction approach
PIC-MCC	combined Particle-In-Cell/Monte Carlo Collision model
QCMD	Quantum-Classical Molecular Dynamics
QCT	Quantum-classical method
QMOCC	Quantum-Mechanical Orbital Closed Coupling
ReaxFF	Reactive force field method and code for CMD calculations
SCC-DFTB	Self-consistent-charge Density Functional Tight-Binding method for QCMD
TC-AOCC	Two-Center Atomic Orbital Close Coupling
TD-DFT	Time-Dependent DFT
UKRMOL	United Kingdom Molecular R-Matrix Code

Experimental

EUV	Extreme Ultraviolet wavelength
FUV	Far-Ultraviolet wavelength
OES	Optical Emission Spectroscopy
PIXE	Proton-Induced X-ray Emission
XPS	X-ray Photoelectron Spectroscopy
PF	Dense Plasma Focus Device

Fusion

α	alpha-particle (^{4}He)
e	electron
p	proton
H	hydrogen
D	deuterium
T	tritium
q	ionic charge
CX	charge-exchange process
ELM	Edge-Localized Mode of fusion plasma
NBI	Neutral Beam Injection heating of fusion plasma

1. Introduction

In the magnetic confinement approach to fusion a deuterium-tritium (D-T) plasma at a temperature of around 15 keV (about 170 million K) is trapped in a magnetic field inside a vacuum vessel. The D-T fusion produces 3.5 MeV α-particles and 14.1 MeV neutrons. Very intense heat flux travels continuously along field lines to material surfaces. Depending on the level of the plasma detachment, temperatures of the particles near the divertor surface are of the order of eV up to 100 eV in steady state conditions. However, in many experiments energy is deposited onto the walls through small or large bursts known as edge-localized modes (ELMs) and disruptions with particle energies in the keV range. Depending on plasma conditions and on the wall material these ELMs and disruptions can lead to evaporation or ablation, potentially causing significant damage to plasma-facing components.

When wall material is rapidly evaporated or ablated a dense expanding plasma cloud may be formed in front of the surface. In this dense plasma the incoming energy may largely be converted from fast particle kinetic energy into radiation energy, and gradient effects may cause this radiation to be directed away from the wall back into the plasma. Energy of photons is more benign to the wall than energy of fast particles, and energy that is reflected back into the plasma is most benign to the wall. This conversion of energy into radiation largely directed away from the material wall is referred to as vapour shielding. The resulted reduction in the energy absorption to the wall surface can be very large; much larger than a simple factor of two that would be expected for isotropic emission of radiation. Continuous vapour shielding has been demonstrated as well, reducing the heat flux to surfaces coated with liquid metals, such as lithium (Li) and tin (Sn), and their mixtures (LiSn).

The heat-load conditions under which vapour shielding will happen depend strongly on the wall material. For D and for easily-ablating wall materials such as Li the process sets in at relatively low heat loads due to the high evaporation rate of Li. For continuous vapour shielding, Li is particularly attractive because relevant steady-state vapour densities can be achieved by controlled evaporation and condensation at moderate temperatures. For tungsten (W) the process is really associated with very high pulsed loads that may occur on fusion experiments and in H-mode plasmas but are difficult to simulate in smaller laboratory experiments. Other relevant materials include beryllium (Be) and steels as possible wall materials, the novel liquid metal target and wall materials Li and Sn, aluminium (Al) because of its use in laboratory experiments as a surrogate for Be, and nitrogen (N), neon (Ne), and argon (Ar) for their use in gas impurity seeding.

Simulation of vapour shielding in some cases involves optically-trapped radiation and requires atomic data such as are used for simulations of hot dense matter: collisional-radiative rate coefficients for ionization and recombination under non-local thermodynamic equilibrium (non-LTE) conditions, and spectroscopically resolved line shapes, opacities and emissivities. The atomic data is needed to simulate the vapour shielding processes and to interpret spectroscopic measurements when vapour shielding is happening, either in transient or steady-state plasma conditions of a fusion device.

The Coordinated Research Project (CRP) on *Atomic Data for Vapour Shielding Processes in Fusion Plasmas* is organized to provide evaluated and recommended data for the principal atomic and molecular processes relevant to vapour formation, and data related to the elemental processes affecting the vapour shielding phenomenon. The primary emphasis is on interactions of hydrogen (H, D, T) with the liquid metal particles being ejected from Li and Sn targets.

The preparatory Consultancy Meeting for the CRP was held on 19 – 20 March 2018 to define the scope of the CRP and the first Research Coordination Meeting (RCM) was held on 13 – 15 March 2019 at the IAEA headquarters in Vienna.

Section 2 summarizes the proceedings of the first RCM and Section 3 summarizes discussions among the participants. In Section 4 are listed the proposed work plans by each CRP group participated the first RCM. The list of participants is presented in Appendix 1 and the Agenda of the RCM is provided in Appendix 2. The summaries of the RCM presentations are listed in Appendix 3. The presentation material for this RCM is found through the web page https://www-amdis.org/meetings/vapour-shielding-rcm1/ .

2. Proceedings

The Head of the Atomic and Molecular Data Unit, C. Hill opened the meeting by welcoming participants and introducing the new personnel of the Unit, K. Heinola as the Atomic Physicist. C. Hill emphasized the background and relevance of evaluated data for vapour shielding processes. The Scientific Secretary of this first Research Coordination Meeting (RCM) K. Heinola, presented the Unit's work and role in the fundamental atomic, molecular and plasma-material interaction data establishment, and in the facilitation of collaborative international research in the production and evaluation of such data for the fusion energy research. The RCM agenda was adopted. Meeting participants introduced themselves and presented their previous and current work, and research plans during the period of CRP. Discussion sessions were arranged after the presentations.

The first day of the RCM comprised of presentations on fundamental modelling activities related to various interaction processes with the plasma and vapour particles. R. Janev presented calculations with Two-Center Atomic Orbital Close-Coupling (TC-AOCC) method on electron (e) capture and excitation in H^+ + Li and H^+ + Sn processes. R. Celiberto described semi-classical and quantum mechanical approaches for calculating vibrational kinetics of electronically excited states in H_2 discharges. I. Bray reviewed the Convergent Close-Coupling (CCC) methodology and its application to e collisions with one-electron (H, β^+, Li, …) and two-electron (He, Be, …) targets. S-B Zhang, a co-worker of Chief Scientific Investigator L. Liu reported results H^+ + Be^+ and Be^{3+} + Li obtained with Molecular Orbital Close-Coupling (MOCC) and TC-AOCC methods as well as free-free transition calculations in H plasma. N. Singh presented relativistic atomic structure calculation results obtained with Configuration Interaction (CI) technique, Multiconfiguration Dirac-Fock (MCDF) method and Flexible Atomic Code (FAC).

The second day focused on computational and experimental activities related to studies on vapour formation properties and vapour spectral analyses. P. Krstić presented results from Classical Molecular Dynamics (CMD) and Quantum CMD (QCMD) simulations of surface effects (chemistry, retention, sputtering) on Li, LiO and C-Li-O targets irradiated with D and D_2 beams. R. Hoekstra presented recent experimental results, methodology and open questions for Sn ion EUV spectroscopy. F. Tabarés presented the OLMAT project for liquid Li metal research and the work plan for vapour shielding physics studies with Neutral Beam Injections (NBI) and laser pulses. M. Akel reviewed the use of Dense Plasma Focus device for the physics studies of vapour formation and its properties using a Sn target. K. Heinola reviewed the Unit's recent activity on the recently launched The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP). After presentations, discussion on the parameters relevant for electronic, ionic and atomic processes in vapour shielding modelling took place.

The third day was dedicated for discussions on the present understanding on the requirements for data and experiments related to vapour shielding phenomena. Each CRP participant reviewed their work plan and discussed how they would contribute to the project until the second RCM which is expected to be held in the second half of 2020. Presentation materials for all the talks are available through the RCM web page https://www-amdis.org/meetings/vapour-shielding-rcm1/.

3. Discussion and Conclusions

Following are notes from the three discussion sessions. In many cases questions are raised for further studies.

General remarks

- Many codes are available for fundamental calculations of electronic, ionic, atomic and molecular processes related to fusion plasma-vapour interactions and for plasma-liquid metal target interactions. The codes or computational methods represented in this RCM are listed in the following. More details on the application of each method are found in Sections 4 and Appendix III. Abbreviations are listed in Section 1.

- CCC: the collision calculations for e + Li collisions have been done outside this CRP and the data will be made available for the CRP's database. The CCC calculations will be extended to p + Li collisions for providing extended CCC data on liquid metal and plasma particles interaction cross-sections. Comparison of the obtained CCC results will be done with other computational methods used within this CRP, such as TC-AOCC and MOCC, which are used for the same collision calculations.
- AOCC and MOCC: the atomic and molecular closed-coupling methodologies will be applied for calculations of ion/atom/molecule processes. Results will be compared with the corresponding CCC calculations on p + Li collisions.
- QMOCC: a fully quantum close-coupling method for ion-atom and ion-molecule collisions. In combination with AOCC method, QMOCC method can be used to obtain high-precision charge transfer cross sections in a broad energy region. QMOCC will be applied to calculate the state-selective electron capture cross-sections for H^+ + Li and H^+ + Sn collisions
- MCDHF, GRASP2K, FAC, CIV3: the Dirac-Hartree-Fock methodologies will be applied for quantum mechanical structural calculations. Also, calculations will be performed on radiative data such as transition energies, and on transition wavelengths, line strength and radiative rates. The elemental species studied include W^{q+} (q = 10 – 25), Be/Fe/Al-like ions, and liquid metals (Li, Sn) and their ions.
- CTMC: Classical Trajectory Monte Carlo Method provides calculations of cross-sections mainly in binary collisions. Results are acceptable when the cross-section is large, usually at the peak of the Bell's curve or for resonant collisions.
- BPRM, DARC: R-matrix codes will be used for calculation of electron impact excitation cross-sections for reactions e + Li^{q+} (q = 0 – 2) as well as e + Sn-ions.
- UKRMOL: R-matrix code is a suite of programs for modeling electron-molecule scattering processes at the state-of-the-art level. In addition to cross-section data, UKRMOL provides also molecular properties (potential curves, dipole moments, etc) as well as resonance parameters required in the characterization of resonant electron-impact processes, such as dissociative attachment, recombination, resonant vibrational excitation and dissociation.
- MRDCI: multi-reference configuration interaction calculations for molecular structures. Using a unique table-CI technique to select important configurations in CI calculation, MRDCI method is used to compute high-precision molecular potential energy curves, coupling matrix elements and transition dipole moments etc, which are important parameters needed in QMOCC calculation.
- MOLPRO: efficient, parallelized molecular electronic structure calculations, which have contributions from many authors. Contains DFT and a library of E C functionals, also Coupled Cluster and Multi-Reference methods. Excited states treated by MCSF/CASSCF, MRCI or FCI, TDDFT, CC and EOM-CCSD. Molecular properties, geometry optimization, vibrational frequencies
- LAMMPS with ReaxFF: combined with EEM is used for fast CMD simulations of plasma interactions with liquid metal surfaces, with inclusion of polarization dynamics. These calculations are to provide additional support, or to replace SCC-DFTB calculations for large systems. Condition to study the systems in this CRP is the existence of relevant Reaxff Bond-Order Potentials (BOP) for Li, Sn, O, H, Mo, W. Most of the required BOPs have been developed outside this CRP.
- SCC-DFTB and DC-DFTB-K are applied for quantum mechanical molecular dynamics (QCMD) simulations when polarization of the material takes place due to presence of Li and/or O. Studied systems comprise of D irradiation of surfaces containing Li, O, C, H. Condition for the use of these methods in this CRP is the existence of Slater-Koster

pair potentials for systems containing consistent mixture of above atomic species, but also Sn, Mo and W. Most of the have been developed outside this CRP, with exclusion of Sn mixtures.

- A requirement was acknowledged for calculations of processes involving molecular collisions with e.g. hydrides such as LiH and SH_4 molecules.
- Experimental data is required for *e* + Sn collisions. A collaboration activity between experimental Sn spectroscopy and fundamental computational methods, such as CCC and TC-AOCC code, will be explored within this CRP.
- There is a special requirement for cross-section line widths and other spectroscopic parameters for experimental Sn spectroscopy with laser-induced ablation. Of special importance is the spectral data for Sn hydrides (SnH_4).
- The effect of hydrogen isotopes in the experiments with Li, Sn, and LiSn was greatly acknowledged. It was discussed to include *p*/D/T in the cross-section calculations.
- Fusion plasma experiments with liquid metals are carried out at TJ-II fusion device. Targets comprise of Li, Sn and LiSn (Li(20%)Sn(80%)). Application of NBI and laser to the targets. The experiments have specific interest on the rate coefficients and will be implementing various cross-sections in plasma confinement of a fusion device. It was stressed, that there is a requirement for an expert performing full particle collision calculations for simulating the plasma-vapour interactions in the fusion environment. This would be to bridge the gap between the fusion experiments and fundamental atomic and molecular calculations.
- Experiments performed with Dense PF device study the vapour formation by exposing Sn targets to ion beams and *e*-beams. Vapour analysis is done by OES and X-ray emission. Further, the vapour elemental composition is studied by analyzing vapour particles being deposited on a secondary target plate.
- Atoms and molecules of interest in relation to this CRP
    - Vapour plasma phase: i) liquid metal elements, their hydrides and other intrinsic impurities, such as Li, Li_2, Sn, SnH_4, LiH, OH, etc. For the time being, Ga was concluded to be excluded from the matrix of studied elements in this CRP due to its corrosive nature making it an impractical candidate as a plasma-facing component material. ii) bulk metal elements mainly for the interest of ITER: W and Be, BeH, BeH_2, etc.
    - Elements on the target surface: Li, LiH, LiOH, Li_2O, SnO, etc. Surface interaction with incoming plasma particles (D, He, D_2,…) yields to erosion of atoms and molecules. However, it is acknowledged that the sputtered molecules likely will dissociate to atoms upon leaving the target surface. Also, the impact molecules are likely to dissociate prior to penetrating the surface. Surface chemistry effects on evaporation, sputtering and retention with a particular focus on the comparison of experimental data with theory.
- Quantities of interest
    - Processes with electron excitations, electron capture, CX between excited charge states of vapour species and H, electron + molecule collisions (resonant and non-resonant)
    - Plasma screening effects to the above processes in dense plasma
    - Ro-vibrationally resolved cross-sections for excitations, charge transfer, ionizations and dissociation, rovibrational energy exchange in atom-diatom collisions
    - Cross-sections for elastic, inelastic, reactive, dissociation (especially LiH and SnH_4), momentum transfer and ionization processes. Requirement for rate coefficients. Special demand for atomic cross-section data for Sn.

- Elastic collision cross-sections for *neutral* + H^+ systems, in particular Li + H^+, Sn + H^+, W + H^+, Be + H^+
- Surface as a source of vapour, processes of sputtering (in particular chemical sputtering), morphology, chemistry, evaporation, implantation and retention, single and multi-component mixtures of Li, SnH, O, C, high-Z substrates (Mo, W), temperature effects

- Energies of interest
  - Steady state plasma conditions of few eVs (from room temperature to 5 eV) up to 100 eV
  - Transient events with few keVs (ELMs, disruptions). While suppression of ELMs by Li is widely accepted, special remark was given, that only few experiments exist which look at ELM suppression on Sn targets. More experimental data is required at transient-relevant energies, e.g. with linear plasma devices, laser ablation, Dense Plasma Focus, *e*-beam experiments.
- Uncertainties and their quantification
  - There is a requirement for establishing uncertainty quantification of the data produced. It was also acknowledged that obtaining good accuracy can be computationally demanding, hence the uncertainties or accuracies may be prioritized for selected computational data. This selection criterion may depend on experimental priorities (e.g. energy specific), which would be a result of close communication between experimentalists and theorists within this CRP.
- Tentative CRP outcome
  - The CRP should provide as an outcome evaluated fundamental computational data on i) *e*, *p*/*d*/*t* interactions with liquid metal elements Li and Sn, and ITER-relevant materials W and Be, ii) collisions with liquid metal molecules, iii) surface processes of liquid metals and the resulted sputtering rates, iv) atomic data of W, Be, Li, Sn.
  - The experimental fundamental work comprises of i) spectroscopic data on Sn, ii) vapour formation and vapour property studies using Li, Sn and LiSn liquid metal targets exposed to fusion plasma, iii) vapour formation and property studies of Sn targets with PF device.
  - All data with their uncertainties will be made publicly available via IAEA repositories
  - The form of the CRP final report will be either a single review publication, a collection of publications, or as an APID volume.

4. Work Plans

Mohamad AKEL, Atomic Energy Commission of Syria (AECS)

- Experiments with Dense Plasma Focus device using bulk Sn as target
- Plasma Focus studies of Sn interactions with plasma ions (He, N_2, Ne, Ar) and *e*-beams
- analysis of the formed Sn vapour using Optical Emission Spectroscopy (OES) and X-ray emission
- analysis and quantification of Sn deposited from the vapour on different substrates using e.g. X-ray photoelectron spectroscopy technique (XPS) and Proton-Induced X-ray Emission (PIXE)
- computation of the generated plasma parameters, such as density and temperature, as well as the ion and electron beam features emitted from the dense plasma focus

Igor BRAY, Institute of Theoretical Physics, Curtin University of Technology

- Collision calculations for few-body systems related to vapour shielding with Convergent Close-coupling (CCC) method.
- Collisional processes of e + Li already calculated and published. Collection of corresponding data and articles for the CRP database.
- Calculations for H^+ + Li ion collisions. Here H^+ represents the hydrogen ionic isotopes *p*, *d* and *t*.
- The CCC method is accurate for energies > 1 keV. Hence for lower energies (< 1 keV) a code comparison activity will be performed against Two-Center Atomic Orbital Closed Coupling (TC-AOCC) calculations performed by Ratko JANEV within this CRP.
- Further CCC code development to incorporate more complicated atomic and molecular targets, such as LiH and Li_2.

Roberto CELIBERTO, Dipartimento di Ingegneria Civile, Ambientale, del Territorio, Edile e di Chimica (DICATECh), Politecnico di Bari

- Calculations of resonant charge-exchange cross-sections for ion-parent atom systems depending on Debye lengths for H, He and Li in the ground and excited states. Work plan for excited states of hydrogen, i.e. $H^* + H^+$, and extension of the method for $He + He^+$ interactions.
- Electron-molecule resonant processes for LiH are calculated: vibrational excitation $LiH + e \rightarrow LiH^- \rightarrow LiH$; dissociative excitation $LiH + e \rightarrow LiH^- \rightarrow Li + H + e$; dissociative attachment $LiH + e \rightarrow LiH^- \rightarrow Li^- + H$ and $Li + H^-$.
- Cross-sections for rovibrational energy exchange in atom-diatom collisions using semi-classical models, like Quasi Classical Trajectory (QCT) method and Quantum Mechanical (QM) methods.
- Self-consistent vibrational kinetics of electronically excited states in H_2 divertor plasma
- Implementation of Particle-In-Cell/Monte Carlo Collision (PIC-MCC) model for the divertor.
- Review of available data of elementary processes for the development of a Collisional-Radiative (CR) model

Ronnie HOEKSTRA, ARCNL

- Review of fusion relevant charge states for Sn
- Experimental measurements for obtaining EUV spectroscopic data of Sn^{q+} (q = 10 – 20) using EBIT. Optical and FUV spectroscopy measurements of intermediately charged Sn^{q+} (q = 3 – 5) with laser-produced plasma source. Analysis of the experimental data performed with theoretical modelling using e.g. CODAN code calculations
- CX experiments with crossed ion beams of Sn^{q+} (q = 1 – 8) and H_2^+ with energy of 0.1 keV/amu.

Ratko JANEV, Macedonian Academy of Sciences and Arts

- AOCC calculations of cross-sections for *e* capture, excitation and ionization in collisions of i) *p* + Li^{q+} (q = 0 – 2), ii) *p* + Be^{q+} (q = 0 – 3), and iii) *p* + Sn^{q+} (q = 0 – 5) in the energy range 1 – 300 keV.
- Cross-section calculations for He^{2+} + Li^+ and He^+ + Sn. Calculation plans for He^+ + Li^+ and He^+ + Sn^+.
- Momentum transfer cross-section and H spectral line intensity calculations for *p* + Li, *p* + Be, and *p* + Sn atoms and ions.
- Collaboration within this CRP with L. LIU (IAPCM, Beijing)
- Comparison of Li results with CCC calculations carried out by I. BRAY within this CRP.

Predrag KRSTIC, Institute for Advanced Computational Science, Stony Brook University

- Sputtering, retention, reflection of D and D_2 of i) Li amorphous surface, ii) fully deuterated Li surface
- Simulation of evolution of the surface layers chemistry and morphology upon evaporative deposition technique of Li and Li_2O layers on Mo substrate
- Deciphering evolution of the oxidation of Li layers; chemistry and temperature dependence
- Solubility and sticking coefficients of D on Li, LiD and Li_2O surfaces

Narendra SINGH, Department of Physics, Shyam Lal College, University of Delhi

- Calculation of electron impact excitation cross sections for reactions *e* + Li^{q+} (q = 0 – 2) as well as *e* + Sn-ions using the R-matrix method
- Structure and transition rates for Sn ions and W^{q+} ions between q = 10 – 25 using GRASP, FAC and CIV3 codes
- Comparison of Li results with CCC calculations done by I. BRAY within this CRP

Francisco TABARES, Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas (CIEMAT)

- The NBI of TJ-II stellarator will be used for irradiating all liquid metal divertor target material candidates at DEMO-relevant high-power densities of 10 – 20 MW/m^2.
- The effect of ELMs to vapour formation will be studied by applying high-power laser pulses during the plasma exposures

- The generated liquid metal vapour will be characterized by emission spectroscopic methods and the resulting plasma plume by Langmuir probes and OES of selected species, such as LiI and LiII.
- The emission of W particles from the liquid metal capillary targets will be monitored to study the effect of sputtered target elements to the vapour formation and shielding efficiency. The effect of the evolution of liquid metal target surface temperature to the vapour formation during NBI exposure will be studied with Pyrometry and Infrared spectroscopy.

Song-Bin ZHANG, School of Physics and Information Technology, Shaanxi Normal University, on behalf of Chief Scientific Investigator Ling LIU, Institute of Applied Physics and Computational Mathematics (IAPCM)

- TC-AOCC calculations for cross-sections of excitation, charge transfer and ionization in collisions between $p + Be^{q+}$ (q = 0 – 3) between energies 1 – 100 keV.
- TD-DFT calculations for total cross-sections of e capture, single and multiple excitation, and ionization for $p + Ne^{q+}$ (q = 0 – 2), and $p + Ar^{q+}$ (q = 0 – 2) between energies 1 – 100 keV.
- Calculations done with collaboration with R. JANEV within this CRP.

Appendix 1

List of Participants

Mohamad AKEL, Atomic Energy Commission of Syria (AECS), 17 Nissan, Kafar Sousah, P.O. Box 6091, DAMASCUS, SYRIAN ARABIC REPUBLIC

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Appendix 2

Agenda

Meeting Room C0229

Wednesday, 13 March 2019

09:30 – 09:50 Christian HILL, Kalle HEINOLA: Welcome, Introduction of participants

09:50 – 10:20 Kalle HEINOLA: Review of meeting objectives, Adoption of agenda

Session 1: Modelling activities

Chair: Kalle HEINOLA

10:20 – 11:10 **Ratko JANEV**, *Macedonian Academy of Sciences and Arts, North Macedonia*
Electron capture and excitation in proton collisions with Li+ and Sn

11:10 – 11:40 Coffee Break

11:40 – 12:30 **Roberto CELIBERTO**, *Polytechnic University of Bari, Italy*
From elementary processes to modelling of low-temperature molecular plasmas

12:30 – 14:00 Lunch

14:00 – 14:50 **Igor BRAY**, *Faculty of Science and Engineering, Curtin University, Australia*
Recent convergent close-coupling progress in atomic and molecular collision theory

14:50 – 15:40 **Song-Bin ZHANG**, *Shaanxi Normal University, China*
Beryllium ion collisions and free-free transition in H plasma

15:40 – 16:10 Coffee Break

16:10 – 17:00 **Narendra SINGH**, *University of Delhi, India*
Relativistic atomic structure calculations with application in fusion plasma

Thursday, 14 March 2019

Session 2: Experimental activities

Chair: Kalle HEINOLA

09:00 – 09:50 **Predrac KRSTIĆ**, *Institute for Advanced Computational Science, Stony Brook University, United States of America*
Surface chemistry, retention and sputtering of solid Li, Li-O and C-Li-O surfaces, irradiated by D and D_2

09:50 – 10:40 **Ronnie HOEKSTRA**, *University of Groningen, Netherlands*
Tin ions: Spectroscopy and interactions

10:40 – 11:10 Coffee Break

11:10 – 12:00 **Francisco TABARÉS**, *Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas, (CIEMAT), Spain*
Studies of vapour shielding physics in the OLMAT facility. Applications to the LMD EuroFusion project

12:00 – 13:30 Lunch

13:30 – 14:20 **Mohamad AKEL**, *Atomic Energy Commission of Syria (AECS), Syria*
Effects of radiation, ion and electron beams emitted from the dense plasma focus on Tin and its alloys

14:20 – 14:50 **Kalle HEINOLA**, *IAEA, Austria*
The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)

14:50 – 15:20 Coffee Break

Session 3: Discussion I

Chair: Kalle HEINOLA

15:20 – 17:00 Discussion (all participants): review of current status of ion-atom collision data and experiments relevant for vapour shielding

19:30 – 22:00 Social Dinner: Gmoa Keller, Am Heumarkt 25, 1030 Wien

Friday, 15 March 2019

Session 4: Discussion II

Chair: Kalle HEINOLA

09:00 – 10:30	Discussion (all participants): Development and review of work plans for the CRP
11:00 – 13:00	Coffee break
11:00 – 13:00	Discussion (all participants): Development and review of work plans for the CRP (cont'd); drafting of the meeting report; adjournment of the meeting

Appendix 3

Presentation Abstracts

Effects of radiation, ion and electron beams emitted from the dense plasma focus on Tin and its alloys

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The dense plasma focus devices have been extensively used as a source of multi-radiation such as neutron yield [1], soft [2] and hard [3] X-rays, ion beams [4, 5], and high-energy relativistic electrons [6, 7]. The low energy (2.8 kJ) Mather-type plasma focus device (AECS PF) is used for material processing as a porous structure [8], bismuth nanospheres, formations on silicon substrates [9] as well as for X-ray radiography [10, 11]. The ion [12] and electron [13] beam features emitted from plasma focus have been computed using Lee model and the energy loss for energetic ions due to interactions with the background gas and target is also calculated using SRIM code [14].

In this work, we are planning to evaporate the Tin targets (pure and alloys) by the plasma focus to simulate the TOKAMAK wall, under various experimental conditions (number of shots, gas pressure, distance from the top of the anode). The sputtered Tin particles (atoms and ions) will be deposited on secondary target (stainless steel substrate or silicon for example). The analysis of this target will give information about the elemental composition of deposited material on the surface of this target. Optical emission spectroscopy measurements of the formed Sn vapour due to interactions of plasma focus (electrons and ions) with the treated targets could be investigated and discussed.

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Recent Convergent Close-Coupling Progress in Atomic and Molecular Collision Theory

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The Convergent Close-Coupling (CCC) method solves Quantum Collision problems in the field of Atomic and Molecular Physics. It is based on the close-coupling expansion of the total wavefunction taken to convergence by utilizing a complete basis. During the 1990s, the CCC method was developed for electron scattering on atomic hydrogen [1], quasi one-electron atoms, which include the alkali metals [2], helium [3] and quasi two-electron atoms, which include the alkaline earths [4]. A relativistic implementation based on the Dirac Equation has also been implemented [5]. These are examples of one-centre problems. The method has been shown to yield accurate results for the major transitions, including differential ionisation, and all incident energies of interest [6].

The CCC method was then extended to two-centre problems such as positron scattering [7] and bare ion scattering [8]. In these cases, electron transfer channel forms the second centre in the problem. Most recently, the CCC method has been extended to molecular targets starting with H_2 [9].

In the talk we will describe the underlying principles of the CCC method and discuss the large variety of recent applications with the goal of modifying the approach to treat problems of interest to the Vapour Shielding Coordinated Research Project.

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From Elementary Processes to Modelling of Low-Temperature molecular Plasmas

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Ionized gas in low-temperature conditions, are in general characterized by the presence of molecular species, which can strongly affect the system properties and its evolution. In particular, when non-equilibrium conditions exists, the interactions occurring among the particles at a microscopic level, give rise to a complex collisional physics, largely dominated by molecules in different internal quantum states which act as different chemical species. So the modeling of these systems requires the characterization of a plethora of collisional processes, involving molecules, where exchanges of ro-vibronic energies, dissociation, ionization, reactive processes etc., may occur. In this frame, the availability of large sets of cross section data becomes a crucial prerequisite for a realistic simulation of plasma system.

In the oral contribution to the present CRP meeting, examples will be given of plasmas of technological interest (ns discharges(1), dense plasmas(2), divertor simulations(3), aerospace entry problems(4)), focusing the discussion on the macroscopic outcomes of the modelling as seen from a point view of the elementary processes. A brief overview on heavy-particle and electron-molecule collisions, will be also presented.

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Tin ions: Spectroscopy and Interactions

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Extreme ultraviolet (EUV) light at 13.5-nm wavelength drives the next generation of nanolithography machines, replacing current technology based on 193-nm light. The step towards EUV is crucial to continue of the miniaturization of the features on chips. Ever since the seventies, the miniaturization is well-represented by Moore's law, predicting the number of transistors on an affordable CPU to double every two years. The shorter the wavelength, the better the resolution, therefore much smaller features can be printed with EUV-based lithography. Highly charged tin ions in plasma of exploding Sn droplets are the atomic sources of EUV light. The transient tin plasmas are of high density with temperatures in the 10-100 eV range.

Spectroscopic information on metal ions in low and intermediate charge states, such as $Sn^{1+ - 20+}$ is very scarce. Interaction cross sections are basically non-existent. At ARCNL we started a collaborative research program on gathering and producing atomic data for tin ions. After a short introduction on ARCNL and laser-produced tin plasma emphasizing the similarities to the outer plasma layers of a fusion device, our work on the spectroscopy of tin ions both in and out of the laser-driven plasma will be presented. A detailed understanding of the complex atomic structure of tin ions is a prerequisite to characterize the plasma. The EUV spectrum of highly charged Sn ions is dominated by intense unresolved transition arrays (UTAs) from the resonance transitions $4p^6\ 4d^m$ -$4p^5\ 4d^{m+1}$ + $4d^{m-1}\ 4f$ in Sn^{8+}-Sn^{14+} [1,2]. The UTAs from serendipitously aligned, strongly interacting configurations from several Sn charge states contribute to a remarkably efficient "in-band" production of 13.5 nm light. Out-off band radiation [3] at shorter wavelength may be used as a diagnostics tool of the "in band" radiation. A side of the EUV spectrum a start has been made to unravel the optical spectrum of tin ions, e.g. Sn^{3+} [4]. Finally I will present first experimental results on charge exchange of tin ions in H2 and on Sn ion scattering on Mo and Ru. The latter results are compared to SRIM simulations showing a remarkable difference in that the single-scattering peak appears to be fully missing in the experiments.

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Electron capture and excitation in proton collisions with Li^+ and Sn

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The results of the research, conducted under the Research Contract No. 23088 within the IAEA CRP on « Atomic and Molecular Data for Vapour Shielding in Fusion Devices », are reported. The processes considered include :

$$H^+ + Li^+(1s^2\ ^1S) \rightarrow H(nl) + Li^{2+}(1s), \quad H^+ + Li^+(1s2s\ ^{1,3}S) \rightarrow H(nl) + Li^{2+}(1s),\ n\geq 2 \qquad (1)$$

$$\rightarrow H^+ + L^+(1s,nl\ ^{1,3}L) \qquad \rightarrow H^+ + L^+(1snl\ ^{1,3}L),\ n\geq 2 \qquad (2)$$

$$H^+ + Sn(\ldots 5s^2 5p^2\ ^{1,3}P) \rightarrow H(nl); \quad H^+ + Sn(\ldots 5s^2 5pnl\ ^{1,3}L),\ n\geq 5 \qquad (3)$$

The computational method used to calculate the cross sections of reactions (1)-(3) was the two center atomic-orbital close-coupling (TC-AOCC) method with large expansion basis sets on each of the centers. The interaction of active electron with the ion cores of Li^+ and Sn was described by spin-dependent 0ne-electron model potentials that reproduce the energies of excited states with accuracy better than 2% in the case of Li^+ states and 7% in the case of Sn states. The coupled equations for the amplitudes of the states included in the AO expansions have been solved by using the straight-line trajectory approximation for the nuclear motion. The accuracy of this approximation in the case of ion-ion reactions (1) and (2) is justified only for energies above 2.5 keV/u.

In the case of reactions (1) and (2) nl-state-selective electron capture and excitation cross sections have been calculated for all states with $n \leq 4$. In the case of reactions (3) state-selective capture cross sections have been calculated for the states with $n \leq 5$, while excitation cross sections were calculated only for the transitions from 5p to 5d, 5f, 6s-6f, 7s and 7p. The oscillator strengths and radiative transition probabilities for these transitions on Sn have also been calculated.

The energy range of calculated cross sections for reactions (1), (2) is 2.5-800keV/u, while for the processes (3) it was 1-300keV/u.

Surface Chemistry, Retention and Sputtering of Solid Li, Li-O and C-Li-O surfaces, irradiated by D and D_2

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Lithium coatings evaporated on a variety of metallic and graphitic surfaces in over ten tokamak fusion machines around the world, has provided evidence of the sensitive dependence of plasma behavior on lithiated plasma facing surfaces [1]. Thus, in NSTX, Li evaporation decreased the H-mode access power threshold, increased the stored energy and allowed longer plasma discharges then for the plasma-facing walls with no Li conditioning [4]. These improvements have been associated with the reduction of impurities and with the reduction of fuel recycling with the formation of Li-O-D complexes.

Our computational studies, a combination of molecular dynamics, quantum physics and computational chemistry modeling [2], extend in spatio-temporal scales not accessible by empirical means and therefore opens the opportunity for a systematic approach at irradiation surface science studies of the plasma-material interface for NSTX and LTX fusion machines. We present our recent theoretical and validating experimental results on the complex surface chemistry processes that evolve from lithium conditioning on plasma-facing materials [3,4,5]. We discuss in details the effects of the lithium coatings at oxidized carbon surfaces to the retention of deuterium and sputtering of the plasma-facing surfaces. The critical role of oxygen in the surface chemistry during hydrogen-fuel irradiation is found to drive the kinetics and dynamics of these surfaces as they interact with fusion edge plasma that ultimately could have critical effects on fusion plasma confinement behavior. The effects of the surface temperature to the retention of deuterium of lithium and lithium-oxide surfaces is also studied [6]. Finally, we report novel data for sputtering, retention and reflection when solid lithium surfaces are irradiated with deuterium atoms and molecules in a wide range of impact energies.

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Relativistic atomic structure calculations with application in fusion plasma

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In the meeting, I will present some of our recent works on relativistic atomic structure which are relevant to fusion plasma research. Fusion research requires accurate and reliable atomic data such as wavelength, energy levels, transition rates, oscillator strengths, etc. These atomic parameters are very fundamental keys for modelling and diagnosis of the plasma for the determination of densities, temperature, etc. in fusion plasmas.

In our work, we have calculated excitation energies or transition wavelengths, radiative rates, oscillator strength, line strength for fifteen Be like ions including Be-like W^{70+}, Ni^{24+} and Sn^{46+} [1-5] which are of particular interest for this project and also studied dependence of plasma parameters on plasma temperature and electron density for hot dense plasmas. The ratio of the intensities of spectral lines within HDP is calculated as a function of electron temperature. For the calculations of energy levels and radiative rates, we have used the multiconfiguration Dirac-Hartree-Fock (MCDHF) method employed in GRASP2K code [6]. The calculations are carried out in the active space approximation with the inclusion of the Breit interaction, the finite nuclear size effect, and quantum electrodynamics (QED) corrections. We have considered valence-valence, core-valence and core-core correlations in our calculations by taking single, double, triple and quartet (SDTQ) excitations. We have also assessed the accuracy of our results and also compared our GRASP2K results with calculated excitation energies from FAC [7] and other theoretical, NIST and experimental results.

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Studies of Vapour Shielding Physics in the OLMAT Facility. Applications to the LMD EuroFusion Project

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The OLMAT-TJII project proposes the use the TJ-II NBI system in order to irradiate Liquid Metal targets with DEMO relevant power densities (neutrals plus occasionally ions), in the range of W< 20MW/m^2.
The targets will be located in a separarted chamber connected to the TJ-II vacuum vessel and facing one of the NBI sources typically used for plasma heating in TJ-II. The nominal power is 1MW at E= 35kV, and the pulse duration is up to 200ms. The repetition frequency for OLMAT experiments can be increased up to 1pulse/2 min. By removing the ion deflectors an extra 30% power can be achieved. In addition, the combined effect of ion irradation and high neutral fluxes can be addressed.
The proposal includes three phases, the first one with some minor modifications to the existing system allowing 200 ms irradiations with 20 MW/m^2, the second one adding a high power laser for transient, ELM-like high power local irradiation and the third one including an upgrade of one of the TJ-II injectors in order to irradiate with long pulses.For the present proposal, phases 1 and 2 apply.
A set of devoted diagnostics is already available, including OES, Langmuir probes, He bem diagnostic, IR cameras, pyrometrs, calorimeter, etc…Some of these diagnostics are already routinely used for beam characterization impigning on a graphite calorimeter. Lithium, and LiSn alloys will be studied, and a lock chamber is attached to the system for easy sample replacement and observation. Actively cooled, refilled samples are being designed for long exposure time experiments.
Vapour shielding effects are expected at these high power densities. They will be characterized by measuring the effective power reaching the sample under different values of the LM temperature. Plasma characterization by the above mentioned diagnostics will allow for the interpretation of the observations and to get insight into the corresponding atomic processes.

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Beryllium ion collisions and free-free transition in H plasma

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In the first part, we will present the studies of state-selective single electron capture, excitation and ionization processes in collisions of H^+-$Be^+(1s^22l)$ and Be^{3+}-$Li(1s^22s)$ [1], by using the quantum-mechanical molecular orbital (QMOCC) and the two-center atomic orbital close-coupling (TC-AOCC) methods in a broad energy range. The total, *n*-shell and state-selective electron capture, excitation and ionization cross sections are calculated with large expansion MO and AO basis sets. In the overlapping energy range the results of electron capture and excitation processes of the two sets of calculations for the main channels agree very well.

In the second part, the free-free absorption Gaunt factors in Hydrogen plasmas are studied by taking into account the plasma screening in the Debye model [3]. It is found that the values of the free-free Gaunt factors for different Debye screening lengths for a given initial electron energy and absorbing photon energy, generally lie between those of the pure Coulomb field and field-free case. However, the Gaunt factors can show dramatic enhancements (broad and narrow resonances) in the vicinities of the critical screening lengths, these enhancements of the Gaunt factors can be significantly higher than their values in the unscreened (Coulomb) case over a broad range. The temperature averaged Gaunt factors are also presented.

The reported results should be useful in the kinetic modeling and diagnostics of edge plasmas in present magnetic fusion experiments, as well as in the current ITER design, in which beryllium is used as first wall material.

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