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Atomic Data for Vapour Shielding in Fusion Devices

Summary Report of the Second Research Coordination Meeting

Virtual Meeting

7–9 October 2020

Prepared by
K. Heinola
IAEA Nuclear Data Section

February 2021

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Abstract

The Second Research Coordination Meeting of the Coordinated Research Project on *Atomic Data for Vapour Shielding in Fusion Devices* was held as a virtual meeting on 7 – 9 October 2020. Eight experts representing eight research institutes globally (Australia, China, India, Netherlands, Spain, Syria, USA) in the field of atomic collisional physics and vapour formation for magnetic confinement fusion devices met together with the IAEA staff. 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 as well as the results obtained. 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.

February 2021

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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

EBIT	Electron Beam Ion Trap
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 plasmas

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. The first Research Coordination Meeting (RCM) was held on 13 – 15 March 2019 at the IAEA headquarters in Vienna and the second RCM was held on 7 – 9 October 2020 remotely as a virtual meeting due to the global SARS-Cov2 pandemic.

Institutes currently participating this CRP represent eight IAEA Member States as listed in https://amdis.iaea.org/CRP/vapour-shielding. Participation of North Macedonia was regretfully discontinued in 2020 due to passing away of the Chief Scientific Investigator of Macedonia Prof. Ratko Janev. Prof. Janev was the head of the A+M Data Unit from 1986 and was an extremely knowledgeable atomic

physicist and a respected colleague who contributed continuously to the field of fundamental data for nuclear fusion. Prof. Janev is greatly missed by the entire plasma physics community.

Section 2 of this meeting report summarizes the proceedings of the second RCM and Section 3 summarizes discussions among the participants. In Section 4 are listed work plans by each of the CRP research group. List of participants is presented in Appendix I and the Agenda of the RCM is provided in Appendix II. The summaries of the RCM presentations are listed in Appendix III and Appendix IV provides the list of publications. The presentation material for this RCM is found through the web page https://amdis.iaea.org/meetings/vapour-shielding-rcm2/.

2. Proceedings

The Section Head of Nuclear Data Section, A. Koning opened the meeting by welcoming participants. He emphasized the importance of vapour shielding processes in fusion reactor environment and the relevance of validated data for the corresponding atomic and molecular processes. The meeting participants introduced themselves. 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.

The first and the second day of the meeting comprised of presentations of the participants focusing to various aspects of vapour shielding in fusion environments. Speaker summaries are provided in Appendix III and presentations are available on the A+M Data Unit web pages at https://amdis.iaea.org/meetings/vapour-shielding-rcm2/.

Kalle HEINOLA (IAEA) described the general status of the Unit's CRPs and reviewed the questions to be addressed in the course of this CRP on Vapour Shielding.

Igor BRAY (Curtin University, Australia) reviewed theory behind the CCC method and presented recent applications of CCC calculations to proton-H and proton-Li scattering calculations. Obtained proton-H cross-sections for electron capture and ionization were compared with computational and experimental results found in the literature. The elastic proton-Li scattering yields to excitation directly which is associated with charge-exchange and breakup. Excitation and electron-capture cross-sections were compared with other works and it was found in the electron-capture process there is split with K-shell and L-shell processes around 100 keV/amu (higher energies dominated by K-shell, lower energies by L-shell interactions).

Ling LIU (Institute of Applied Physics and Computational Mathematics (IAPCM), China) discussed the results obtained with QMOCC, AOCC and TDDFT methods. The total and state-selective charge transfer and excitation cross sections are obtained for H^+-Be collisions using QMOCC and AOCC. The recommended charge transfer data has been given in the energy range between 0.1 – 100keV/u. The excitation, ionization and charge transfer cross section data for H^+-Ne^{2+}/Ar^{2+}/Ne^{7+}/Ne^{8+} collisions have been presented by using the AOCC and TDDFT methods, and it is found that for the high charged targets the excitation is the dominated process and the cross sections for other processes are much smaller. Using the AOCC method, the reliable total and state-selective cross section data for H^+-H(*2l*) collision has been obtained in the energy region 0.1-100 keV/u, and the electron is dominantly captured to *2l* states.

Narendra SINGH (University of Delhi, India) presented atomic data for Sn ions (Sn^{3+} and Sn^{4+}) and W ions (W^{11+} and W^{13+}) as obtained with FAC. Calculated properties were energy levels, transition wavelengths, oscillator strengths and transition rates. Discrepancies in excitation energies and transistion wavelengths of Sn3+ and Sn4+ as wells as properties of fine-strcucture splitting of Sn3+ were discussed. Also, these theoretical findings predict the lifetime for fine structure levels $4d^9 5s$ to be extremely large. Transition data for the lowest 304 and 500 fine structure levels of W^{11+} and W^{13+}, respectively, have been calculated. The theoretical results obtained were compared with other theoretical works and experimental results and discrepancies were discussed.

Ronnie HOEKSTRA (University of Groeningen, The Netherlands) discussed the structure and interactions of medium-charge Sn ions ($q < 20+$) as observed in the EUV range. EBIT was deployed in reconstruction of charge-state resolved spectra of Sn ions. Importance of doubly-excited levels was reviewed. The EBIT spectroscopy for EUV emission of Sn^{15+} and Sn^{16+} requires deconvolution analysis due to the spectra being a mix of various other charge states: deconvolution is a necessity for a clean charge state resolved spectra. It was pointed out the need for understanding and reliable theoretical calculations of stopping and charge exchange processes of Sn ions propagating in H_2 gas.

Predrag KRSTIĆ (Stony Brook University, United States of America) reviewed the properties and chemistry of Li surfaces and oxidized Li surfaces and their interaction processes with fusion plasmas. Describing plasma-Li-wall interactions requires fundamental atomistic and nano science. For theoretical research, MD simulations have been applied for the studies Li surface sputtering with and without surface impurities (O, C) under the bombardment of D and D_2 projectiles in the energy range from 5 – 100 eV. It was found the D retention to decrease and the Li sputtering to increase as the D impact energy increases. Similar trend was observed with Li:D surfaces, but with a higher overall retention. However, the Li_2O surface showed significantly higher D retention and lower sputtering than the clean Li surface. Effect of Li and Li:H surface temperature was not found to play a crucial role in H sticking to the surface.

Bruce KOEL (Princeton University, United States of America) described the experimental investigations on fundamental processes and synergistic effects in plasma-material interactions relevant to fusion energy. Research focus is on liquid metal plasma-facing components and include studies of energetic hydrogen and deuterium atoms, ions, and molecules with liquid and solid films of Li, Sn, and Li-Sn alloys. Close collaboration and benchmarking experiments with computational group by Predrag KRSTIĆ was reviewed.

Francisco TABARÉS (Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas (CIEMAT), Spain) presented the current status of the OLMAT facility and corresponding results obtained. OLMAT is in the assembling phase and first experiments are expected by the end of 2020 or early 2021. Wetting issues of liquid metals in tungsten porous supports have been solved and incorporated to the target design. The attenuation of Li and Sn atoms in TJ-II hot plasmas has been measured at different LM temperatures. Together with edge characterization by the He beam diagnostic, it has allowed for the estimate of the kinetic energy of the corresponding atomic species (Li, Sn) release from the target as a function of its temperature. Qualitative agreement with the thermal sputtering model was found for Li. The deduced energies for tin atoms are a factor up to 30 times higher than those expected according to the Thomson model, thus indicating an overestimation of the ionization rate constant for tin by a factor of 5.

Mohamad AKEL (Atomic Energy Commission of Syria, Syria) presented the application of Mather-type low energy (2.8 kJ, 15 kV, 54 kA) plasma focus (PF) device AECS-PF1, which is used for deposition of the tin alloy (60%Sn+40%Pb) on the intrinsic silicon (111) substrates under different

conditions: distance from the top of the anode (3, 4, 5, 6, 7 cm) and number of shots or discharges (5, 10, 15). The plasma focus discharge is operated in nitrogen and argon gases at a pressure of around 0.8 mbar. SEM, EDX and XPS techniques have been used for analysis of the silicon treated samples. SEM images show that the size of deposited particulates from the anode materials have different dimensions and distribution according to the used number of plasma shots (the size becomes bigger with higher shots). At different distances from the top of the anode, it is noticed that the amounts of elements decrease with increasing distance up to 7 cm and the size of deposited particulates are smaller at further distance from anode. Variation of atomic concentration (%) on the treated substrates as a function of etching time (0, 10, 25 and 50 min) has been demonstrated using XPS. The five-channel diode x-ray spectrometer (DXS) is also assembled and installed on plasma focus device to obtain the x-ray emissions from plasma and targets. The present results of DXS show that there is no x-ray emission from PF device at the current operational conditions and the parameters optimization is going on.

The Lee model code has been also applied on the plasma focus device. The used plasma focus parameters and the properties of electron as well as ion beams are determined for all experiments. The corona model has been also used as an approximation for computing the thermodynamic data of the tin plasma generated in the plasma focus. Based on the obtained plasma temperature range (100 – 130 eV) in plasma focus device, the expected tin ionization fractions to be generated during the pulse pinch plasma focus are up to Sn^{+18}, Sn^{+19}, Sn^{+20}, Sn^{+21}.

3. Discussion and Conclusions

The third day of the meeting was devoted to discussions and conclusions. Participants agreed that there is a need for theoretical predictions at atomistic and corresponding atomic-level data level to increase the confidence of experimental finding. Uncertainty quantification is crucial in determination of the boundaries of errors. Code-code comparison, experimental collaborations and other joint activities will be supported within this CRP.

Selected 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 and the details on the application of each method are listed in the meeting report of the first RCM of *Vapour Shielding* CRP. The meeting page of the first RCM is online https://amdis.iaea.org/meetings/vapour-shielding-rcm1/ and the corresponding meeting report can be found at https://www-nds.iaea.org/publications/indc/indc-nds-0781/ .
- CCC calculations (I. Bray) 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 have been extended to p + Li collisions for providing extended CCC data on liquid metal and plasma particles interaction cross-sections. It was acknowledged need for comparing the CCC results against corresponding results obtained with semiclassical AOCC and MOCC methods (L. Liu) used within this CRP. This code-code comparison would begin with analyzing results from state-resolved p + H processes incl atomic and excited states, transitions and ionizations. Next stage will be comparing results for the p + Li processes with a number of Li excited states.
- R-matrix calculations will be used for calculations of electron impact excitation cross-sections for reactions e + Li^{q+} (q = 0 – 2) and for e + Sn ions (N. Singh). A cross-comparison activity for e + Li results obtained using CCC will be established. It was noted, that e + Sn system is too complicated to be assessed with CCC. However, ionization, excitation and metastable stats of Sn can be approximated by CCC making it valuable for plasma experiments. It was also discussed, that e + Sn^{q+} experiments with q = 1 – 2 could be performed within this CRP (R. Hoekstra).

- Critical component in the simulations of Li surface interactions with classical MD is a reliable interatomic potential (P. Krstic). Complexity of Li systems arise from the dynamic electron cloud of Li. Requirement for an MD potential describing accurately the polarization effects due to activity in the electron cloud was addressed. Currently there is only one open source potential for Li, which is a ReaxFF Bond-Order Potential and implemented in the LAMMPS code. However, a new computational tool DC-DFTB-K opens possibility for quantum mechanical calculations for large atomistic systems and its capability for Li should be explored. A good test case for code comparison of ReaxFF and DC-DFTB-K would be a Li system with O and H. It was stressed, that calculations for large Li systems should be always validated by experiments (B. Koel): current Li simulations with MD are cross-checked with experimental studies as a joint research project. MD simulations provide qualitative features, whereas experiments provide quantitative information. This synergy is especially important in studies with surfaces and interfaces and at low impact energies.
- Interatomic potential for Sn is well established. There is need for a Li-W potential for simulating e.g. Li targets with W capillary systems.
- At TJ-II stellarator experiments are ongoing in which pure Sn and LiSn mix samples are exposed to fusion plasma (T. Paco). Also, LiSn samples are being prepared for laboratory studies with ion beams and TDS (B. Koel). High-intensity Plasma Focus device has been used for exposing Sn alloys to study the formation and properties of Sn vapour (M. Akel).

- In the first RCM a requirement was acknowledged for calculations of processes involving molecular collisions with e.g. hydrides such as LiH and SnH_4 molecules. The current RCM presented the first results for e + LiH calculations. Requirement for SnH_4 calculations was reviewed and it was concluded, that those may be postponed or fully omitted. This is motivated by the SnH_4 property to get decomposed at 100 ˚C resulting to SnH_4 molecules not being survived in fusion plasmas.

- Highly ionized Sn is more relevant to processes taking place in the core of fusion plasma. For vapour shielding processes at the plasma edge or SOL, information and data is required for low-q Sn ions (up to Sn^{4+}).

- More experimental data is needed for fuel retention in Li, LiO and LiD surfaces and lattices. Further, information on the transition from Li sputtering to Li evaporation is lacking. MD simulations can be used to study the evaporation process in addition to the conventional sputtering research.

- There is a continuous requirement for experimental data for e + Sn collisions. A collaboration activity between experimental Sn spectroscopy, Dense Plasma Focus experiments and fundamental computational methods, such as CCC and TC-AOCC code, will be explored further within this CRP.

- Requirements for cross-section line widths and other spectroscopic parameters relevant for experimental Sn spectroscopy with laser-induced ablation were discussed.

- The relevance of the isotopic effect of hydrogen in experiments with Li, Sn, LiSn was discussed. The importance of isotopic effect was acknowledged for retention, sputtering and vapour formation, however, the corresponding experimental challenges remain. Isotopic effect will be studied in the theoretical cross-section calculations e.g. with CCC.

- Experiments with Dense Plasma Focus device will seek the possibility of creating plasmas with light gases.

4. Work Plans

Mohamad AKEL (Atomic Energy Commission of Syria, Syria)

- Study and analysis of the deposited Tin structures by plasma focus operated with different gases (Helium, Neon and argon)
- Measurement of X-ray emissions from plasma focus device with the presence of the Tin targets
- Analysis of the formed Sn vapour using Optical Emission Spectroscopy
- Simulation of the generated plasma focus parameters for all experiments

Igor BRAY (Curtin University, Australia)

- CCC method has been implemented for scattering of electrons, positrons, photons and antiprotons on quasi one- and two-electron targets as well as inert gases
- Proton-Li scattering implemented in a one-center approach
- Inclusion of calculations of $H+He^+$, $H+H_2^+$, $H+Ne^+$ and other inert gas ions
- Inclusion of molecular targets X_2, H_2O and other

Roberto CELIBERTO (Polytechnic University of Bari, Italy)

- Extension of the study of the electron-impact excitations involving LiH and Li_2 molecules. In particular, for the optically allowed transition $(X^1\Sigma^+) \rightarrow (A^1\Sigma^+)$ the so-called EV cross sections will be derived to estimate the role of the indirect mechanism of vibrational excitation of the ground state through the singlet excited state.
- The highest electronic states will be also considered and the ab initio electronic structure calculations of the corresponding potential energy curves are in progress for the singlet terms of the electronic spectrum of LiH molecule.
- The Li_2 electron impact excitation and dissociative excitation through excited electronic states will be investigated by semi-classical and simplified approaches.
- The electronic structure calculations of the lithium dimer, at a MRCI level with standard gaussian basis set, are in progress for the derivation of the adiabatic potential energy curves of the ground $\left(X^1\Sigma_g^+\right)$ and of the singlet excited states, $(^1\Sigma_u^+)$.

Ronnie HOEKSTRA (University of Groeningen, The Netherlands)

- Studies of mitigation of Sn ions coming from the plasma (resulted Sn charge distribution, ionic energy spectrum, interactions with H_2 gas, generation mechanism of Sn ions, etc)
- Collisional processes of Sn ions with H_2 gas
    - Charge exchange, ionization, stripping, stopping power in H_2, energy loss/gain
    - Processes with H_2, $[H_2]^+ \rightarrow H_2^+$ or $H^+ + H$ and $[H_2]^+ \rightarrow H^+ + H^+$
    - Upgrades to the experimental facility
        - H2 gas jet replaced with H source
        - Upgrade to the Faraday Cup and Thomson Parabola Spectrometer for low-resolution stopping and straggling measurements
        - High-resolution energy loss measurements with Class 100 spectrometer

Predrag KRSTIĆ (Stony Brook University, United States of America) and **Bruce KOEL** (Princeton University, United States of America)

Computational plan (P. Krstić):

- Isotopic effects (H, D, T) in sputtering and retention of hydrogen at hydrogen molecules at Li layers
- Sputtering and retention of hydrogenic species of Li_2O surfaces as a function of substrate temperature (25 – 220°C) and energy of incident particles (1 – 100 eV) (H, D, T)
- Sputtering and retention of hydrogenic species of LiOH surfaces as a function of substrate temperature (25 – 220°C) and energy of incident particles (1 – 100 eV) (H, D, T)
- Effects of the surface structure on the sputtering and retention of H off monocrystal and amorphous surfaces (Li, LiH, Li_2O)
- Hydrogen sticking coefficient at oxidized lithium layers and its dependence on temperature

Experimental plan (B. Koel):

- Continue surface science investigations of simple model systems under well-controlled conditions to obtain additional fundamental experimental data, with experiments designed to benchmark and connect to ab initio theory and simulations.
- Studies of the thermal stability and hydrogen uptake, retention, and sputtering of Li, Sn, and Li-Sn alloy films on several high Z substrates, e.g. Mo, TZM, and W, and the influence of oxygen and carbon contamination on these processes. These studies will utilize high resolution XPS and vibrational spectroscopy to better characterize the chemical state of the Li films and the roles played by LiOH and Li_2O in these processes. In addition, we will utilize a Colutron differentially pumped ion source capable of mass tuning for ion species selection that was recently equipped with an electrostatic deceleration lens system for ion energies in the hyperthermal regime down to a few eV. Thus, new ion beam studies of D^+ ion – Li interactions will be conducted with incident ion beams of 10 – 1000 eV.
- A HIDEN Ion Desorption Probe quadrupole mass spectrometer with ion optics & a retarding field will be used to detect neutral species and positive and negative ions, and their energies, to investigate incident ion reflection and retention, and understand Li erosion and the physical or chemical sputtering mechanism. Our goal is to convert these signals into quantitative information on yields.

Ling LIU (Institute of Applied Physics and Computational Mathematics (IAPCM), China)

- Electron capture, excitation and ionization cross section calculations for H^+-Be^{2+} and H^+-Be^{3+} collision systems by using the AOCC method;
- Electron capture, electron loss and ionization cross section calculations for H^+-$Ne^{(4, 5)+}$ and H^+-$Ar^{(4, 5)+}$ collision systems by using the TDDFT method.

Narendra SINGH (University of Delhi, India)

- Calculations of fine structure energies and radiative data such as transition energies, transition wavelengths, line strength, oscillator strength and radiative rates (transitions/wavelengths required)
    - W and Sn ions using GRASP and FAC
- Calculations of atomic data for Li ions

- Studies of atomic processes and calculations of electron impact excitation cross-section and photoionization cross-section of W, Sn and Li ions

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

- Exploitation of the OLMAT facility in its 1st phase. Studies of Vapor shielding effects on Li and Sn targets
- Acquisition and coupling of a powerful fiber laser to the OLMAT facility for ELMs simulation studies.
- TJ-II experiments of LM insertion for atomic data validation of Sn atoms and Sn^{+} ions at Te values from 5 to 50 eV.

Appendix I: List of Meeting Participants

Mohamad AKEL, Atomic Energy Commission of Syria, Syria

Igor BRAY, Curtin University, Australia

Ronnie HOEKSTRA, University of Groeningen, The Netherlands

Predrag KRSTIĆ, Stony Brook University, United States of America

Bruce KOEL, Princeton University, United States of America

Ling LIU, Institute of Applied Physics and Computational Mathematics (IAPCM), China

Narendra SINGH, University of Delhi, India

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

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Appendix II: Meeting Agenda

Second Research Coordination Meeting on "Atomic Data for Vapour Shielding in Fusion Devices" (Virtual)

Wednesday 07 October 2020

Welcome (13:00-13:20)

Welcome, Introduction of the participants, Agenda, Remarks from RCM1

- Arjan KONING, Kalle HEINOLA, Christian HILL

Fundamental modelling and theories: Discussion 1 (13:20-14:20)

13:20	Calculation of proton-lithium scattering using the CCC method	BRAY, Igor Curtin University, Australia
13:50	Hydrogen, Helium and Lithium plasmas: from the dynamics of elementary processes to modelling of fusion devices	CELIBERTO, Roberto Politecnico di Bari, Italy

Virtual coffee (14:20-14:40)

Fundamental modelling and theories: Discussion 2 (14:40-15:40)

14:40	Electron capture, excitation and ionization in collisions of Be, Neq+, Arq+ ions with proton	LIU, Ling Institute of Applied Physics and Computational Mathematics, China
15:10	Excitation energies, radiative data and collisional excitation cross-section of Sn (Sn3+, Sn4+) and W (W11+ and W13+) ions	SINGH, Narendra University of Delhi, India

Thursday 08 October 2020

Experiments and simulations: Discussion 3 (13:00-14:00)

13:00	Medium-charged Tin Ions structure and interactions	HOEKSTRA, Ronnie University of Groningen, The Netherlands
13:30	Surface chemistry, retention and sputtering of solid Li, Li2O, LiH surfaces, irradiated by H and H2	KRSTIC, Predrag Stony Brook University, USA KOEL, Bruce Princeton University, USA

Virtual coffee (14:00-14:20)

Experiments and simulations: Discussion 4 (14:20-15:20)

14:20	OLMAT Contribution to the 2nd RCM of Vapor Shielding CRP	TABARÉS, Francisco CIEMAT, Spain
14:50	Effects of radiation, ion and electron beams emitted from the dense plasma focus on Tin and its alloys	AKEL, Mohamad Atomic Energy Commission of Syria, Syria

Friday 09 October 2020

Review and summary: Discussion 5 (13:00-14:30)

Virtual coffee (14:30-14:50)

Review and summary: Discussion 6 (14:50-16:20)

Appendix III: Summaries of Presentations

Calculation of proton-lithium scattering using the CCC method

Igor Bray[1]

Co-authors: Ilkhom Abdurakhmanov; Corey Plowman; Alisher Kadyrov

[1] *Curtin University*

We review the convergent close-coupling (CCC) method for calculating collision processes in atomic and molecular physics, concentrating on systems with heavy projectiles such as proton-atom scattering. Particular attention is paid to the one- and two-center approaches to the problem. More specifically, we will discuss the proton-lithium scattering results recently published by Abdurakhmanov et.al., J. Phys. B, 53, 145201 (2020).

Hydrogen, Helium and Lithium plasmas: from the dynamics of elementary processes to modeling of fusion devices

Roberto Celiberto[1]

Co-authors: Ratko Janev; Annarita Laricchiuta

[1] *Politecnico di Bari, Italy*

One of the problems arising in thermonuclear fusion research, is represented by the excessive thermal load on plasma facing components of fusion devices, coming from the intense heat flux reaching the material surfaces. A possible strategy, aimed to the reduction of the thermal exposure, is represented by the use of liquid metals, which, after evaporation, leads, through interaction with the main plasma, to the conversion of the thermal energy in radiation, which is finally dispersed in the plasma bulk. This conversion process reduces the heat flux on the reactor walls, generated by the particle impacts, thus preventing the thermal degradation and chemical erosion of the material components. Among the many candidates for vapour shielding, lithium is considered one of the most promising metals.

After evaporation, the lithium atoms present in gas phase, can give rise to reactive processes which can yield to the formation of molecular species, like Li2 dimers or LiH hydrides. These molecules, animated by internal rovibronic motions, can play a non-negligible role in the conversion of internal energy in radiation. A general mechanism for radiative processes involving molecules, is represented by the excitation of the internal states by particle collisions, followed by photon emission. Typical example is given by the so-called radiative decay which can be represented by the following two-step process (also known as E-V process) [1]:

$$M_2(X,v) + e \rightarrow M_2(A,v'') + e \rightarrow M_2(X,v') + e + \hbar\omega \qquad (1)$$

In the first step the diatomic molecule, M_2, in one of the vibrational levels of its ground electronic state, (X,v), is excited by electron impact to the spectroscopically allowed vibro-electronic state (A,v''), followed by the decay again in the vibrational manifold of the ground state, included the dissociative continuum, through the emission of a photon with frequency ω. The calculation of the cross section for this process requires the electron-impact cross section data for the first step, as well as the emission Einstein coefficients for the second. Experience acquired with other electron-molecule scattering systems, shows that both these quantities heavily depend on the initial vibrational excitation of the molecule.

A theoretical modeling, aimed to the simulation of the best conditions for an efficient vapour shielding in fusion plasmas, must include, thus, the description of the vibrational kinetic for a realistic determination of the time-dependent vibrational population of all molecular species acting in the plasma. The very first step for the construction of such model, starts from the knowledge of the collision cross sections for vibrational energy exchanges of molecular species with all the other particles present in the system.

In our group, we have started the calculations of electron collision cross sections involving vibrationally excited LiH. In particular, cross sections and rate coefficients have been calculated for the vibro-electronic transition $\mathrm{LiH}(X1\Sigma+,v) + e- > \mathrm{LiH}(A1\Sigma+,v') + e$, by using a modified form of the Mott and Massey scattering approximation [2]. The complete dataset has been derived for the excitations from the 24 vibrational levels of the ground state. The state-to-state cross sections for the $v \rightarrow v' = v$ excitations display a significant increase with the vibrational energy content (see Fig.1), reflecting the behavior of the transition dipole moment with the stretching of the molecular bond. Moreover, analytical functions have been derived that accurately reproduce the energy profile of the cross sections for their easy implementation in kinetic models.

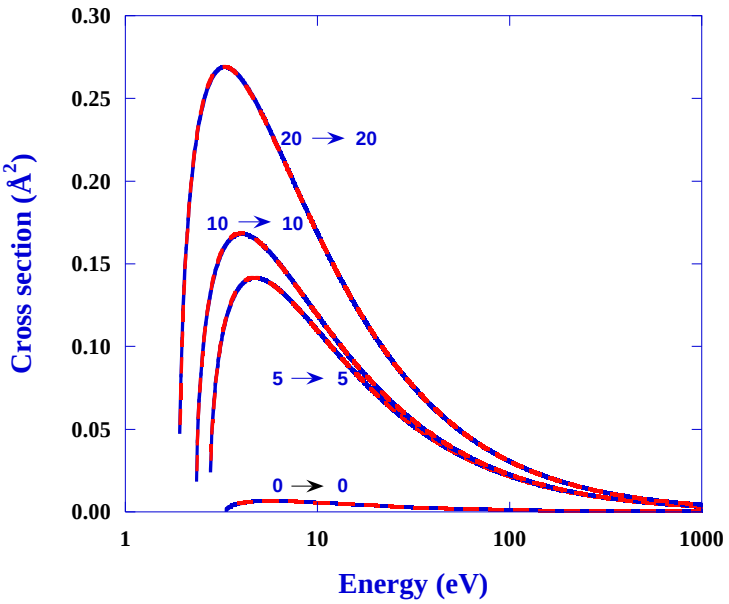

Fig.1 Electron-impact cross sections for the $v \rightarrow v' = v$ excitations. Full-blue line: calculated crosssections; dashed-red line: analytical fits. Reproduced from Ref. [2]

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Electron capture, excitation and ionization in collisions of Be, Ne^{q+}, Ar^{q+} ions with proton

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The electron capture and excitation processes in H^+-Be collisions are investigated by the quantum mechanical molecular orbital close-coupling (QMOCC) method and by the two-center atomic orbital close-coupling (TC-AOCC) method in the energy range 1-1000eV/u and 0.5-100keV/u, respectively. Total, n-shell and state-selective electron capture and excitation cross sections are calculated with large expansion of MO and AO basis sets. In the overlapping energy range the results of the two sets of calculations are compared. Meanwhile, collisions of proton with $Ne^{1,2+}$ and $Ar^{1,2+}$ ions are studied using the time-dependent density-functional theory (TDDFT). The electron capture, electron loss and ionization cross sections are obtained in the energy range of 1-100keV/u and compared with data from other sources when available.

Excitation energies, radiative data and collisional excitation cross-section of Sn (Sn^{3+}, Sn^{4+}) and W (W^{11+} and W^{13+}) ions

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We have calculated atomic data such as energy levels, transition wavelengths, oscillator strengths, and transition rates for Sn^{3+}, Sn^{4+}, W^{13+} and W^{11+} ions [1,2]. We have employed Flexible atomic code (FAC) in our computations. We have computed lowest 31, 17, 304 and 500 fine structure levels for Sn^{3+}, Sn^{4+}, W^{11+} and W^{13+}, respectively. We have provided transition data among lowest 31, 17, 304 and 500 fine structure levels for Sn^{3+}, Sn^{4+}, W^{11+} and W^{13+}, respectively. We have calculated lifetime of Sn^{3+} and Sn^{4+} ions and compared with theoretically calculated and experimentally measured lifetimes. We have also predicted that lifetime of fine structure levels of $4d^9 5s$ is extremely large and can be used as metastable states. We have also reported collision cross-section for Ag-like and Pd-like Sn from ground state to lowest 31 levels and 17 levels, respectively. We have compared our calculated data with available theoretical and experimental results [3-12] and discussed difference between them.

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Medium-charged Tin Ions structure and interactions

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In this talk our progress on identifying and characterizing multiply charged tin ions, structure, charge state, kinetic energy, and their interactions with stopping gas and plasma-facing materials surrounding a laser-produced plasma (LPP) extreme ultraviolet (EUV) light source is presented.

The following topics will be addressed:

- EUV line identifications in medium-charge Sn ions using reconstructed charge state resolved spec-tra from an electron beam ion trap (EBIT).
- The double-magic structure of Sn ions underlying the efficient generation of 13.5 nm EUV light inSn LPP EUV sources.
- Optical depth as a single, pertinent scaling-law parameter capturing the overall trends in the observed changes in the complex EUV emission of the Sn LPP plasma.
- Time- and space-resolved optical Stark spectroscopy in the afterglow of the LPP plasma.
- Sn ion interactions with solid material (Ru, Mo) towards improvement of the predictive power ofthe commonly used SRIM simulation package.
- Aspects of stopping and charge exchange interactions of Sn ions traversing H_2 gas.

Surface chemistry, retention and sputtering of solid Li, Li-O, C-Li-O surfaces, irradiated by D and D_2

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[2] Princeton University, USA

Conditioning with lithium has led to improved performance in a variety of experimental fusion machines [1]. These improvements have been associated with the reduction of impurities and the reduction of fuel recycling with the formation of Li-O-D complexes [2]. 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 profound effects on fusion plasma confinement behavior.

In the 2nd year of this CRP we continue our theoretical and experimental studies on the lithium and lithium hydrogenated and oxidized surfaces irradiated by hydrogenic particles (ions, atoms, molecules), having in mind conditions at the fusion boundary plasma, primarily of NSTX and LTX machines in the Princeton Plasma Physics Laboratory. Our computational studies [3], based on molecular dynamics, quantum physics, and surface chemistry modeling, were devoted to understanding the fundamental processes in particle-surface interactions and obtaining data for retention, sputtering, reflection, and sticking coefficients. We report on the novel data for these processes in the range of impact energies 0.025 to 100 eV at amorphous Li and L2O surfaces. The effects of the surface temperature were also studied at Li surfaces [4].

Experimental studies of the plasma particle interactions with lithiated surfaces have a double role: to inspire detailed computational approaches for explanations of the data and to validate results of the computational modelling. We report on the use of temperature programmed desorption (TPD) in ultra-high vacuum experiments to investigate the effects of temperature on hydrogen (H) or deuterium (D) retention in pure Li and Li_2O films [4], sputtering of Li-C-O compounds under D^+ ion bombardment [5], and the post-exposure time-dependence of D retention in Li and Li compounds [6]. In characterizing the initial Li film, we found that the Li thermal stability increased by 350 K upon oxidation with O_2, H_2O, or CO. Both Li and Li_2O were comparable in efficiency in retaining H, but H is retained as LiH in pure Li until LiH decomposition leads to Li and H_2 desorption after heating to 650 K. It appears that LiOH is formed after an Li_2O film was irradiated with H^+ ions and decomposed to Li_2O and H_2O above 470 K. The Li-O sputtering rate is lower than Li-C-O and it peaks at a higher energy of 800 eV D^+.

We also used TPD along with other surface diagnostics to study both clean and oxidized Li and Sn films on a TZM molybdenum alloy [7]. Sn films and the Sn monolayer are more thermally stable by 600 K than corresponding Li films, e.g. complete Sn evaporation from TZM does not occur until 1700 K. Oxygen impurities affect the thermal stability of Li and Sn films very differently, e.g. oxidation increases Li stability by 400 K, while it decreases Sn stability by 200 K. Finally, we report some preliminary data and describe upcoming experiments using an ultralow energy ion beam to study H^+_x − Li interactions over the range of 10 − 1000 eV by monitoring the emitted species and their energies to measure low energy incident ion reflection and retention, and understand Li erosion and the physical or chemical sputtering mechanism.

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OLMAT Contribution to the 2nd Research Coordination Meeting of Vapor Shielding CRP

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- During the last year, the OLMAT facility has been designed and built at CIEMAT. First plasma ex-periments are planned by the end of 2020, conditioned to the restrictions imposed by the COVID-19 crisis.
- Activities at the lab have focused on developing liquid metal targets of Li and Sn with good wettingproperties and proper support by the metallic capillary system.
- Some activities in TJ-II in relation to the Task were also undertaken. The kinetics of atomic Li and Sn species released from the CPDS system by their interaction with the TJ-II hot plasma were investigates and conclusions about their binding energy and ionization rate constant were driven. It was found that the ionization rate constant of Sn atoms by electron impact has been largely overestimated in the bibliography

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

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Mather – type low energy (2.8 kJ, 15 kV, 25μF, 54 kA) plasma focus (PF) device is used for deposition of the tin alloy (60%Sn+40%Pb) on the intrinsic silicon (111) substrates under different conditions: distance from the top of the anode (3, 4, 5, 6, 7 cm) and number of shots or discharges (5, 10, 15). The plasma focus discharges are operated in nitrogen and argon gases at a pressure of around 0.8 mbar. The analysis of silicon treated targets demonstrates that the amounts of both elements decrease with increasing distance up to 7 cm from the anode. SEM images show that the size of deposited particulates from the anode materials have different dimensions and distribution according to the used number of plasma shots. Variation of atomic concentration (%) of Sn, Pb and N as a function of etching time are found using XPS technique. Five channel (BPX65 PIN) diode x-ray spectrometer (DXS) is also assembled, installed and tested on PF device to investigate x-ray emission properties of the hot dense plasma. The obtained signals of DXS reveal that there is no x-ray emission from AECS-PF1 device at the present operational parameters.

The computational program Lee model (RADPFV5.15FIB&REB) is applied on the PF device working in nitrogen and argon in order to simulate the realized experiments. The used PF parameters and the properties of electron as well as ion beams (flux, heat flux, current, fluence, energy fluence, number of electrons, energy in beam, damage factor, etc..) are determined for each shot. The corona model has been also used as an approximation for computing the thermodynamic data of the tin plasma generated in the plasma focus. The ion fraction, effective ionic charge number and effective specific heat ratio for tin plasma have been calculated at different temperatures. Based on the obtained plasma temperature range (100 – 130 eV) in PF device, the Sn^{18+}, Sn^{19+}, Sn^{20+}, Sn^{21+} ionization fractions are expected to be generated during the pinch plasma.

Appendix IV: Publications

List of publications as a result of this CRP

I. B. Abdurakhmanov, C. Plowman, A. S. Kadyrov, I. Bray and A. M. Mukhamedzhanov, "*One-center close-coupling approximation to two-center rearrangement collisions*", J. Phys. B: At. Mol. Opt. Phys. **53**, 145201 (2020)

R. Celiberto, R. K. Janev and A. Laricchiuta, *Electron-impact state-to-state cross sections and rate coefficients for X(v)→A(v') excitation of LiH molecule,* Plasma Sources Sci. Technol., **29**, 035008 (2020).

Z. Bouza, J. Scheers, A. Ryabtsev, R. Schupp, L. Behnke, C. Schah, J. Sheil, M. Bayraktar, J. R. Crespo López-Urrutia, W. Ubachs, R. Hoekstra and O. O. Versolato, "*EUV spectroscopy of Sn^{5+}-Sn^{10+} ions in an electron beam ion trap and laser-produced plasmas*", J. Phys. B: At. Mol. Opt. Phys. **53**, 195001 (2020)

J. Scheers, C. Shah, A. Ryabtsev, H. Bekker, F. Torretti, J. Sheil, D. A. Czapski, J. C. Berengut, W. Ubachs, J. R. Crespo López-Urrutia, R. Hoekstra, and O. O. Versolato, "*EUV spectroscopy of highly charged Sn^{13+}-Sn^{15+} ions in an electron-beam ion trap*", Phys. Rev. A **101**, 062511 (2020)

L. Liu, C. H. Liu, J. G. Wang and R. K. Janev, "*Electron capture and 2s-2p excitation in Be^{3+}-Li collisions*", Journal of Quantitative Spectroscopy & Radiative Transfer **242**, 106804 (2020)

L. Liu, C. H. Liu, J. G. Wang and R. K. Janev, "*Electron capture, excitation and ionization in H^{+}-Be^{+} collisions*", Eur. Phys. J. **D73**, 200 (2019)

M. X. Ma, B. H. Kou, L. Liu, Y. Wu and J. G. Wang, "*Electron capture in collisions of Li^{3+} ions with ground and excited states of Li atoms*", Chinese Physics B **29**, 013401 (2020)

N. Singh and A. Goyal, "*Energy levels, transition data and collisional excitation cross-section of Sn^{3+} and Sn^{4+} ions*", J. Electron Spectros. Relat. Phenomena **244**, 146982 (2020)

N. Singh, S. Aggarwal and M. Mohan, "*Extended atomic structure calculations for W^{11+} and W^{13+}*" Atoms **8**, 92 (2020)

A. Devitre E. Oyarzabal, I. Fernandez-Berceruelo, D. Tafalla and F.L. Tabares, *"Boron synergies in lithium-film performance"*, Nucl. Fusion, **60**, 106001 (2020)

Publications relevant to this CRP

F. Torretti, J. Sheil, R. Schupp, M. M. Basko, M. Bayraktar, R. A. Meijer, S. Witte, W. Ubachs, R. Hoekstra, O. O. Versolato, A. J. Neukirch and J. Colgan, "*Prominent radiative contributions from multiply-excited states in laser-produced tin plasma for nanolithography*", Nat. Comm. **11**, 2334 (2020)

R. Schupp, F. Torretti, R.A. Meijer, M. Bayraktar, J. Scheers, D. Kurilovich, A. Bayerle, K.S.E. Eikema, S. Witte, W. Ubachs, R. Hoekstra, and O.O. Versolato, "*Efficient generation of extreme ultraviolet light from Nd:YAG-Driven microdroplet-Tin plasma*", Phys. Rev. Applied **12**, 014010 (2019)

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J. Scheers, R. Schupp, R. Meijer, W. Ubachs, R. Hoekstra, and O. O. Versolato, "*Time- and space-resolved optical Stark spectroscopy in the afterglow of laser-produced tin-droplet plasma*", Phys. Rev. E **102**, 013204 (2020)

A. de Castro, A. Sepetys, M. González and F. L. Tabares, "*Temperature dependence of liquid lithium film formation and deuterium retention on hot W samples studied by LID-QMS. Implications for future fusion reactors*", Nucl. Fusion **58**, (2018)

F. L. Tabarés, D. Alegre, M. Baldwin, D. Nishijima, M. Simmonds, R. Doerner, E. Alves, R. Mateus, "*Studies of lithium deposition and D retention on tungsten samples exposed to Li-seeded plasmas in PISCES-A"*, Plasma Phys. Control. Fusion (2017) DOI:10.1088/1361-6587/aa5bae

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