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Atomic Data for Vapour Shielding in Fusion Devices

Summary Report of a Consultancy Meeting

IAEA Headquarters, Vienna, Austria

19–20 March 2018

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IAEA Nuclear Data Section

July 2018

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Report prepared by
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IAEA Nuclear Data Section

Abstract

A Consultancy Meeting was held on 19–20 March 2018 at IAEA Headquarters in Vienna to review atomic data needs for simulations of vapour shielding in fusion devices and to delimit the scope of a possible coordinated research project on that topic. The proceedings and discussions during the meeting are summarized here.

July 2018

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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 toroidal magnetic field inside a vacuum vessel. Very intense heat flux travels continuously along field lines to material surfaces. Furthermore, in many experiments energy is deposited onto the walls through small or large bursts known as edge-localized modes (ELMs) and disruptions. 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 is 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 largely directed away from the wall back into the plasma. Energy in photons is more benign to the wall than energy in 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 reduction in energy to the 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, Sn and Li.

In fusion devices, vapour shielding is also associated with the process of pellet injection: the injection of high-velocity pellets of frozen deuterium or of certain impurities into the hot plasma. Deuterium pellets may be injected for plasma fuelling and “killer” pellets of frozen argon or neon may be injected to quench a discharge at an incipient disruption. For certain diagnostic purposes hydrogen (deuterium) pellets seeded with an impurity have been injected in plasma experiments. The physics of vapour shielding for pellet ablation is similar to that of wall material.

The heat-load conditions under which vapour shielding will happen depend strongly on the wall or pellet material. For deuterium and for easily-ablating wall materials such as lithium the process sets in at relatively low heat loads. For continuous vapour shielding, lithium is particularly attractive because relevant steady-state vapour densities can be achieved by controlled evaporation and condensation at moderate temperatures. For tungsten the process is really associated with very high pulsed loads that may occur on fusion experiments but are difficult to simulate in smaller laboratory experiments. Other relevant materials include beryllium and iron as possible wall materials, gallium and tin in connection with liquid metal walls, aluminium primarily because of its use in laboratory experiments (as a surrogate for beryllium or just for basic diagnosis studies), and nitrogen, neon, and argon for impurity pellet injection.

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. Following advice from the International Fusion Research Council (IFRC) Subcommittee on Atomic and Molecular (A+M) Data the A+M Data Unit is planning to start a Coordinated Research Project (CRP) on atomic data that are needed to simulate vapour shielding or needed to interpret spectroscopic measurements when vapour shielding is happening, either in transient or steady-state conditions.

The present report is the output of a two-day Consultancy Meeting on atomic data for vapour shielding that was held at IAEA to review the state of atomic data and data needs for vapour shielding studies and to make recommendations about the scope and objectives of the planned CRP. These recommendations will form the basis of a proposal to the IAEA Committee on Coordinated Research Activities (CCRA) to initiate the planned CRP with a start date in Q1 2019.

Section 2 summarizes the presentations at the meeting. Section 3 summarizes the discussions and conclusions. Appendix 1 provides the list of participants and Appendix 2 the meeting agenda. Appendix 3 provides speaker summaries of the presentations. Appendix 4 presents the conclusions of the CM in the form of a proposal to CCRA to initiate a CRP on atomic data for vapour shielding. Finally, Appendix 5 lists recent relevant journal literature from the fusion community related to vapour shielding and recent relevant conference contributions at major fusion meetings.

2. Presentations

Speaker summaries are provided in Appendix III and presentations are available on the A+M Data Unit web pages at https://www-amdis.iaea.org/CRP/VapourShielding/CM/.

The meeting was opened and participants introduced themselves. **Christian Hill** (IAEA) described the general nature of CRPs and their role in the Agency programme and reviewed the questions to be addressed in the course of this CM.

Dr Goldston (Princeton Plasma Physics Laboratory) presented some recent simulation results modelling a lithium vapour box divertor. The box divertor, in which lithium evaporates and recondenses within a baffled (partially-enclosed) volume has been proposed as a means of continuously shielding the fusion reactor surfaces from the high heat flux entering the scrape-off layer (SOL) in a tokamak, whilst minimizing the amount of impurity ions that enter the core plasma. Whilst most aspects of the vapour transport in these models are well-accounted for by Monte Carlo techniques, there remain uncertainties in the atomic physics. In particular, data is sought on the interactions between lithium in multiple charge states, electrons, hydrogen ions, and molecular species such as H_2 and LiH. Much of this data is missing from the major databases used in the field, ADAS and ALADDIN.

Particular questions that need to be addressed:

- How much energy is lost from the upstream plasma due to lithium influx?
- What are the mechanisms of detachment with high Li content?
- Is photon opacity at the relevant densities of a box divertor an issue in understanding its mechanism?
- Can the behaviour of hydrogen inside the condensed lithium be modelled?

Dr Krasheninnikov (UCSD) discussed inertial and dissipative models of vapour shielding. Both models potentially use fundamental atomic data (in the first case in the determination of the collisional transfer of energy to the vapour cloud, and additionally in the second case by taking into account radiative losses from the cloud). Radiation trapping effects (due e.g. to the hydrogen Lyman lines) may play a role here, but it is noted that the commonly-used EIRENE code does not include radiation trapping in its treatment of radiation transport.

Dr Morgan (DIFFER) described recent experiments on vapour shielding carried out using his institute's linear plasma devices Magnum-PSI and Pilot-PSI. The power conducted to a tin surface in these experiments was found to be reduced by vapour shielding effects by a factor of about a third, and there is a clear oscillatory signal in the resulting surface temperature caused by the interaction between slow thermal cooling effects and fast plasma processes. Direct evaporative losses of Sn are not a major factor in vapour shield protection, which appears to be dominated by the ion recombination to neutrals which removes momentum directed at the strike point. However, the necessary data for Sn (cross sections for charge exchange between Sn and H^+, He^+, electron-impact excitation for Sn^{z+} (z=0-5), and momentum exchange (particularly between Sn and H) are sparse. It is hoped that the proposed CRP can address this need for evaluated, relevant atomic data for tin.

Dr Peschanyy (KIT) and **Dr Pitts** (ITER) discussed their modelling of the behaviour of tungsten tokamak divertor targets under transient heat loads using the TOKES code. When vapour shielding of the W target is taken into account through ionization of the ablated material, the degree of damage (as measured by melt depth and surface area) is predicted to be significantly reduced. Accurate atomic data is thought to be relatively unimportant for assessing the extent of wall damage, but is known to be important for modelling the size and behaviour of the vapour cloud itself. There is a particular interest here in the properties of medium charge states of tungsten (W^{10+} - W^{25+}) which are found to be responsible for the majority of re-radiation of the transient energy pulse (at least in the optically-thin regime thought to be appropriate for ITER-like conditions). In addition to ion line data, key processes are ionization, recombination, excitation rates It was openly admitted that it would be desirable to include ADAS data into TOKES, but manpower is lacking to perform this task.

The TOKES results have been benchmarked against plasma-gun experiments on W (using the MK-200UG and 2MK-200 facilities) and can hopefully help evaluate the atomic data used in these vapour shielding models. It is, however, recognized that within any such simulation code, the atomic data used is intrinsically linked to the modelling of the plasma dynamics.

Pellet ablation (particularly that of deuterium-doped neon or pure argon pellets, the planned options for ITER disruption mitigation) also requires similar atomic data for its accurate modelling. Dielectronic recombination rates are particularly poorly understood in this context.

Dr Scott (LLNL) described his group's work on radiation-hydrodynamic and collisional-radiative modelling of vapour shielding. Both low and high density regimes require "full" atomic models, though the need for detailed structure in the radiative properties of atomic species is less important at high densities because of collisional broadening. Non-LTE workshops are found to be very useful in identifying requirements for atomic models. It was noted that whilst line shapes are important for diagnostics (e.g. in relation to Stark effect analysis), they are not as relevant, for example, to the assessment of divertor target damage in tokamaks. There remains a lack of evaluated data for several atomic species, especially Sn but even for Li (when there is the need to consider a large number of dielectronic recombination channels). Although there is a real lack of evaluated data, the codes are now powerful enough so that we can calculate a lot of atomic data with very good confidence. The exceptions are for near-neutral stages of mid- to high-Z elements and the details of complex multi-electron n=4 stages where configuration interaction is very important, but even these cases are becoming approachable.

Questions posed in relation to this presentation included:

- What are the expected density and temperature ranges for which to set appropriate model parameters?
- Which molecular reactions can occur?
- Do non-thermal electrons pose a role?

As always, it will be helpful to compare experimental data and simulations where possible.

3. Discussion and Conclusions

The second day of the meeting was devoted to discussions and conclusions. Participants agreed that a CRP on Atomic data for vapour shielding in fusion devices is timely. The discussions focussed on the scope and aims of the proposed CRP in the area of development, evaluation and recommendation of atomic data and on the roles within the CRP of atomic physics, radiation trapping, plasma modelling and experiments with ablating and continuously evaporating materials.

It is important to note that the CRP is to be focussed on the provision of evaluated atomic data for vapour shielding applications. We cannot address issues such as plasma dynamics, divertor design or the methodologies for the calculation of ablation rates, except in so far as they rely on fundamental atomic data.

The questions addressed by the CM, and the conclusions of their discussion are given below.

- What kinds of atomic data are needed to diagnose and to simulate vapour shielding in general? "Kinds of data" can encompass spectroscopic data (lines and line shapes), effective (CR) ionization and recombination rate coefficients (atomic kinetics), opacities and emissivities, and maybe equations of state.
    - o Atomic and Molecular data:

        - Ionization, recombination, charge exchange (CX), rovibrational excitation (for molecules), momentum transfer (especially for ion-neutral systems);
        - Opacities; collisional (de-)excitations, spontaneous emission; modelling of charge states when many autoionizing states are required;
        - Line parameters including line shapes and the influence of Stark and Zeeman effects;
        - Collisional processes between atomic and molecular hydrogen and materials of interest (see below);
        - Cross sections for particle-in-cell (PIC) kinetic modelling (especially for W-plasma interactions), as adopted by the ITER organisation (R. Pitts, D. Tskhakaya).
    - Methodologies for data reduction in the context of large line lists used for radiation trapping modelling
        - Further study is required to determine the importance of radiation trapping in W plasmas (i.e. what is the optical thickness of such plasmas?)
        - It should be established whether it is feasible to take a line-by-line approach, to adopt some kind of averaging (as described by S. Peschanyy), or to use photon absorption cross sections (opacities). The importance of photon reabsorption is therefore also relevant in this context.
- Are there any data needed for diagnostics (spectroscopy) that are not also needed for simulation?
    - It was noted the fine structure is often needed for modelling.
    - The data needs for vapour shielding simulation should be informed as far as possible by interaction with experimentalists.
- Which materials should be considered in connection with this CRP? Should the CRP be dedicated to plasma-material interaction with the divertor and wall material, or should pellet ablation (for fuelling pellets and “killer” impurity pellets) also be considered?
    - Conventional first wall and divertor materials: W (ITER divertor), Be (ITER first wall), Fe / Steel (DEMO first wall, ITER port plugs), Al (a proxy for Be). The primary interest here is for transient events rather than the “steady-state”/continuous plasma operation;
    - Liquid metals for continuous and transient vapour shielding: Li, Sn, Ga
        - Data is also required on LiH, SnH_4, Li_2, and other relevant molecules.
        - Species formed between Li and impurities such as O, C and N are poorly understood and potentially of interest within this CRP.
    - Although relevant, high-quality data concerning Ar and Ne (as used in “killer” pellets) is thought to be already available in the ADAS database and elsewhere, this should be confirmed.
- What role, if any, should the provision of data for the modelling of the behaviour of liquid metal walls have within the CRP? In particular, should fundamental data (including charge-exchange with H/D/T) concerning Li, Sn (and maybe Ga) be in scope?
    - It was agreed that the provision and evaluation of data concerning the vapour shielding offered by liquid metal walls both in continuous plasma operation and during transients should be within the scope of this CRP.
- To what extent should the CRP concern itself with (thermally-enhanced) sputtering and the effect of surface chemistry on sputtering and evaporation?
    - For surface chemistry, the influence of hydrogen co-deposition on sputtering and evaporation is thought to be important and data in this area are sparse.
    - It is noted that an improved model for thermally-enhanced sputtering is required.
- What emphasis should be placed on the provision of atomic data (particularly opacities) for H, D or T?
    - The conclusion of discussions on this was that all of the relevant data were known to acceptable accuracy.
- Can present data on e.g. ablation be used to validate atomic / spectroscopic data?

    - For pellet ablation: the interaction between plasma modelling and fundamental atomic data is complex.
    - There is data from a JET experiment on W-melting under ELM loading still to be analysed.
    - Facilities actively producing relevant data in this area are: Magnum PSI / Pilot PSI (plasma gun at DIFFER), MK-200UG (plasma gun at TRINITI), under a contract with the ITER Organization to be launched in mid-2018, with first results expected in early 2019, with the University of Hyogo (fast transient ablation experiments with Al), PISCES-B (laser ablation experiment at UCSD), electron beam ablation (Novosibirsk and Budker Institute of Nuclear Physics), QSPA Kh-50 (plasma accelerator at Kharkov)
- Are there any other activities that the Atomic and Molecular Data Unit might initiate to support the objectives of the CRP?
    - Code comparison activities, particularly in the area of autoionization and dielectronic recombination models.
    - Groups providing experimental data for the validation and comparison of models should be identified.
- What is the scope for coordinated research amongst participating groups, including code comparison and benchmarking, and the validation of calculated data against experiment?
    - There is scope for relevant comparison activities here, give suitable participation from the appropriate research groups. Important codes in the area of vapour shielding simulation are: SOLPS-ITER, TOKES (S. Peschanyy, KIT), HEIGHTS (Purdue), the simulation code of K. Ibano (U. Hyogo), EIRENE (FZJ), and B2.5-EUNOMIA (DIFFER)
    - Important codes in the area of atomic data calculation are: FAC, ADAS, HULLAC, the LANL Atomic Physics Code Center, GRASP2K, and SONIC.
- With respect to production of atomic data, what is the proper role of dense plasma electronic structure theory (e.g. based on TD-DFT) in this CRP and what is the proper role of atomic structure theory with plasma effects? What is the role of non-LTE model development?
    - These activities were deemed to be outside the scope of this CRP.

It was agreed that there is considerable scope for coordinated research within the terms of this CRP, particularly in the areas of benchmarking data and codes against experiment, code comparison, and in the investigation of the radiative properties of vapour shields. Whilst the data needs of the “traditional” fusion tokamak community and those working on liquid metal divertor designs are different, there are some areas of crossover, particularly in the study of the radiative properties of plasma vapours. The concern of the former community for shielding under transient events and that of the latter for the continuous shielding properties of liquid metal components is noted.

The proposal narrative for the CRP under consideration at this meeting is given in Appendix IV.

Appendix I: List of Participants

R. J. Goldston, Plasma Physics Laboratory, Princeton University, Princeton, NJ, USA.

S. Krasheninnikov, Center for Energy Research, University of California at San Diego (UCSD), La Jolla, CA, USA.

T. W. Morgan, Dutch Institute for Fundamental Energy Research (DIFFER), Eindhoven, NETHERLANDS.

S. Pestchanyi, Karlsruhe Institute of Technology, GERMANY.

R. A. Pitts, ITER Organization, Saint Paul-lez-Durance, FRANCE.

H. A. Scott, Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA.

C. Hill, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

Appendix II: Meeting Agenda

Consultancy Meeting on "Atomic Data for Vapour Shielding in Fusion Devices."

Monday 19 March 2018, Room A2311

09:30 C. Hill: *Welcome and Introduction*

10:00 R. J. Goldston: *The Lithium Vapor Box Divertor*

10:30 S. Krasheninnikov: *My View on the Vapour Shielding Issues*

11:00 *Coffee Break*

11:30 T. W. Morgan: *Liquid metal vapour shielding in linear plasma devices*

12:00 S. Peschanyy and R. A. Pitts: *Plasma shielding during transients on ITER*

12:30 Discussion

13:00 *Lunch*

14:00 H. A. Scott: *Data requirements for simulating vapor shielding with radiation-hydrodynamic and collisional-radiative modeling*

14:30 Discussion: *Scope of the CRP, atomic data requirements, which materials should be considered?*

15:30 *Coffee Break*

16:00 Discussion *(continued)*

17:00 End of Day One

19:00 Evening Meal

Tuesday 20 March 2018, Room A2311

09:00 Discussion: *Possible coordinated research activities and data evaluation activities*

11:00 *Coffee Break*

11:30 Discussion: *CRP outcomes: databases, code and data comparison exercises, and recommendations*

13:00 Lunch

14:00 Discussion: *Potential CRP participants, draft timetable for the CRP*

15:30 *Coffee Break*

16:00 Final Remarks and Review

16:30 Close of meeting.

Appendix III: Summaries of Presentations

Introduction, meeting objectives

C. Hill

International Atomic Energy Agency

This presentation briefly summarises the history of the IAEA's Atomic and Molecular Data (AMD) Unit, its activities and place in the organisation. The nature and purpose of Coordinated Research Projects (CRPs) is described and the procedure for initiating one outlined. Typical activities related to a CRP such as code comparison and benchmarking activities are discussed and currently active and recently completed CRPs are briefly described.

The questions for the present Consultancy Meeting to consider in the preparation of a proposal for a CRP on Vapour Shielding in Fusion Devices are outlined (see Section 3 of this report), the participants introduced, and the meeting agenda adopted.

The Lithium Vapor Box Divertor

R. J. Goldston, E. Emdee, J. Schwartz

Plasma Physics Laboratory, Princeton University, Princeton, NJ, USA

Recent experimental and theoretical analyses indicate that even the quiescent scrape-off layer in a tokamak reactor plasma will have too high a power density to be delivered to a material surface. Solution to this problem is likely to require radiation in the scrape-off layer. However the same narrow SOL width that makes the heat flux high also reduces the radiating volume of the SOL. Furthermore, it is crucial that a minimum of impurities be introduced into the main plasma.

We have developed, therefore, a concept for a lithium vapor box divertor, in which lithium evaporates and recondenses in a partially isolated volume, dramatically reducing the impurity gas influx to the main plasma. It is also very robust against changes in the heat flux from the plasma, since as the divertor plasma “dips its toe” more deeply into the vapor cloud, its absorption of lithium strongly increases. In calculations for an FNSF plasma we find a factor of 4 increase of impurity absorption for ~ 5 cm deeper penetration into the vapor cloud. We have approximated the needed parameters for such a vapor box using a “cooling per ionized atom” model, and a Direct Simulation Monte Carlo code for the vapor transport. The results are encouraging, but the atomic physics of the interactions between lithium in multiple charge states, electrons, and D T ions, atoms and molecules requires clarification. Furthermore, evaporation and condensation on capillary porous surfaces filled with (impure) lithium requires further elucidation.

My View on the Vapor Shielding Issues

S. Krasheninnikov

University California San Diego, La Jolla, CA 92093, USA

There are different models of the vapour shielding. In a ballpark they could be divided on two major categories: i) inertial models, and ii) dissipative models. These models are very different and involve different atomic physics effects.

The first one is relying on inertial heating of the vapour cloud (ablated material) by incoming heat flux, which is carried by plasma particles. The amount of energy reaching the surface is determined by the stopping power of the vapour. No dissipation of energy from the vapour is accounted for. As an example of such model one could refer to the shielding of pellets (both H and impurity) (e.g. see Ref. 1-3).

The second one, in addition to the heating of the vapour cloud, involves also dissipation of incoming heat flux by the radiation loss. For example: shielding of dust particles in tokamak edge plasma, and impact of large ELMs and disruption on divertor targets, and, finally, effective "impurity and hydrogen shield" of divertor targets in detached regimes (e.g. see Ref. 4-6). We notice that in the latter case the radiation trapping effects (e.g. Hydrogen Lyman lines) play an important role (e.g. [7, 8])

We show that atomic physics data used in different approaches to vapour shielding problem is intrinsically linked to particular plasma model implemented. We discuss major atomic physics processes relevant to different shielding mechanisms and demonstrate that comparison of simulation results with experimental data requires careful choice of comparing parameters [9].

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Liquid metal vapour shielding in linear plasma devices

T.W. Morgan[1], G.G. van Eden[1], P. Rindt[2], V. Kvon[1], D. U. B. Aussems[1], M. A. van den Berg[1], K. Bystrov[1], N.J. Lopes Cardozo[2] and M. C. M. van de Sanden[1]

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[2]*Eindhoven University of Technology, 5612 AZ Eindhoven, The Netherlands*

Liquid metals used in plasma facing components are attractive for DEMO due to the liquid's ability to self-heal against erosion, immunity to most of the negative impact of neutrons and ability to go beyond conduction-only based cooling. One extension of this cooling is vapour shielding, occuring under high heat loading of the liquid-metal surface by the plasma leading to strong evaporation. In such a situation the interaction between the vapour and the plasma leads to additional energy and momentum loss which reduce the power to the surface from the plasma by these additional volumetric processes. A series of experiments carried out in DIFFER's linear devices Magnum-PSI and Pilot-PSI have explored this phenomenon in detail for the first time. These machines are able to recreate the high density ($>10^{20}$ m^{-3}) low temperature (<5 eV) conditions expected close to the partially detached strikepoints of ITER or DEMO. It was found that the surface temperature of Sn based substrates becomes locked when the plasma pressure and vapour pressure become similar, and that this temperature locking persists over a power input range of 1-20 MW m^{-2}. Due to ion-neutral friction and electron ion collisions the plasma is strongly cooled from 2-3 eV to <0.5 eV driving strong recombination. The plasma cooling and radiation leads to an overall reduction of ~one third in the conducted power. Additionally the process appears oscillatory in nature due to the mutual interaction of the thermal cooling (slow) with the plasma processes (fast). For Li similar behaviour is also observed and appears a general phenomenon which would be expected to be present in tokamaks. The talk will discuss vapour shielding for liquid metals and the needs for atomic data to give a deeper physical understanding and predictive capabilities for these processes.

Plasma shielding during transients on ITER

S. Pestchanyi[1] and R. A. Pitts[2]

[1] *Karlsruhe Institute of Technology*

[2] *ITER*

Simulations using the TOKES fluid code transient heat loads on ITER, in particular those expected during unmitigated major disruptions have shown that significant target melt damage can be expected on the tungsten (W) divertor targets. Although, every effort will be made to minimize the number of such events on ITER through the use of prediction, avoidance and mitigation strategies, they cannot be completely avoided, particularly in the early years of ITER operation when these strategies are being developed. These TOKES results also show, however, that, when plasma shielding due to ionization of the vapourized W material is included in the simulations, the degree of damage (in terms of melt depth and the melted surface area) can be reduced by several factors in comparison with the unshielded case,. The plasma energy released in the transient is converted into radiation inside the shielding layer close to the target and the radiation redistributes the energy onto the surrounding wall more evenly than the disruptive plasma itself does. Code results indicate, importantly, that the vapour shielding effect switches on at comparatively low transient energy density, so that some plasma shielding benefit may already be derived early on in the ITER experimental program when unmitigated disruption and edge localized mode transients will be more frequent.

The talk will describe key aspects of the TOKES code [1] relevant to the modelling of shielding and show first the results of code benchmarking against 2MK-200 plasma gun experiments on W [2], followed by examples of application to ITER divertor target transient loading [3]. Further plasma gun experiments, currently being planned in Russia under a contract with ITER and which will also be benchmarked against TOKES, will be mentioned and would hopefully contribute to the future vapour shielding CRP. The ITER simulations clearly show the importance of taking into account the 2D nature of the target interaction and show that the majority of re-radiation of the transient energy pulse is ascribed to medium W charge states (e.g. W^{10+} - W^{25+}) and may be described with acceptable accuracy in an optically thin approximation. Accurate optical data is important for correct simulation of the amount of vapourized material, but less important for simulation of solid wall damage. The talk will highlight those areas in which atomic data is missing, with key elements being accurate data for W ion lines (particularly medium charge states), ionization and recombination rates as well as the excitation rate coefficients for all ions.

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Data requirements for simulating vapor shielding with radiation-hydrodynamic and collisional-radiative modeling

H. A. Scott, *Lawrence Livermore National Laboratory*

The phenomenon of vapor shielding relies on the interaction of energetic particles with a vapor layer to convert kinetic energy into radiation. We consider simulating this process on a macroscopic scale with a radiation hydrodynamics code driven by a collisional radiative (CR) model for material properties. The CR model needs a complete set of atomic data, but the required extent of that data depends greatly on the physical conditions encountered during the simulation. We focus on those microscopic interactions between radiation and vapor which are important to radiation transport and discuss the effects of trapped radiation on material properties and energy balance. Example materials will include hydrogen, lithium and tin.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Appendix IV: Core of Proposal for a CRP on Vapour Shielding

The formal proposal to initiate a CRP follows a certain template. What follows are the key narrative sections.

Scope and aims of the CRP

An activity by the A+M Data Unit on vapour shielding would be concerned with the production, evaluation and recommendation of atomic data relevant for vapour shielding in fusion devices. These atomic data include non-local thermodynamic equilibrium (non-LTE) collisional radiative transition rates, line shapes, opacities and emissivities. The relevant atomic species are those foreseen as first wall and divertor plasma-facing materials, and perhaps also hydrogen and impurities used in pellet injection scenarios. Under conditions of vapour shielding basic atomic energy levels and transition rates are modified by the dense plasma environment; therefore, the CRP is concerned with atomic data for warm and hot dense matter.

The application domain of nuclear fusion motivates priorities among the atomic species, but the applications are not a part of this CRP. The CRP does not have direct objectives to estimate ablation rates for wall or pellet material or to assess the viability of various plasma scenarios or device designs that involve vapour shielding.

The most important atomic species for attention in the CRP are those of tungsten (as a divertor target material), the liquid metals lithium, gallium and tin, main wall materials beryllium and iron (steel), hydrogen (deuterium) fuelling pellets and nitrogen, neon and argon killer impurity pellets. In addition, aluminium is important due to its use in well-controlled laboratory experiments as a surrogate for Be or just for basic well-diagnosed studies.

In addition to concrete objectives in the production, evaluation and recommendation of atomic data this CRP will also have an important role in bringing together atomic physicists with expertise in warm and hot dense matter with plasma modellers and plasma spectroscopists that study vapour shielding in fusion devices and in controlled laboratory conditions. Theoretical studies and modelling activities in the fusion community tend to focus on plasma effects, for example associated with the electrostatic sheath, and to use rather simple models for the atomic physics. The CRP must contribute to the transfer of atomic data and associated expertise into the plasma modelling activities related to vapour shielding.

Relation to other CRPs

The Atomic and Molecular Data Unit has coordinated three CRPs in recent years on plasma-material interaction in fusion devices, each for one specific class of relevant materials.

- CRP F43020 on Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials (2012-2016).
- CRP F43021 on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices (2013-2018).
- CRP F43022 on Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices (2015-2020).

These three earlier CRPs are concerned with material erosion and with tritium retention in fusion materials under routine plasma exposure. On the other hand, the proposed new CRP on Vapour Shielding is concerned with extreme heat load events leading to strong ablation and evaporation of wall material. The study of such extreme events involves different experimental and theoretical approaches. The main point of contact with these earlier CRPs is the shared interest in plasma-material interaction.

Nuclear Component

The processes considered in this CRP have a key role in nuclear fusion experiments and in future nuclear fusion devices including ITER.

CRP Overall Objective

To support fusion energy research in Member States by providing trusted data for atomic processes relevant to vapour shielding in fusion plasma, and thereby to contribute to the development of fusion energy generation.

Specific Research Objectives

Recommend elastic collision cross sections for neutral-H^+ systems, in particular Li + H^+, Be + H^+, Al + H^+ and W + H^+.

Assess the importance of and, if appropriate, assemble evaluated data relating to charge-exchange between (excited) charge states of vapour species and H.

Assess the effect of tungsten vapour opacity in transient shielding, as modelled by various codes, including TOKES.

Assemble, evaluate and recommend relevant atomic data (in particular, momentum transfer (differential) cross sections, other collisional cross sections and rate constants) for Sn.

Assemble data relating to the interactions of LiH and SnH_4 with plasma species at energies down to room temperature (0.025 eV). Particularly relevant data are: ionization, (rovibrational) excitation, charge-transfer, elastic collisions; dissociation (especially for LiH). With lower priority, collect and evaluate data relating to interactions between Li, LiH and H_2 with the impurity species C, O and N.

Assess surface chemistry effects on evaporation and sputtering, with a particular focus on the comparison of experimental data with theory.

As far as possible, attempt experimental validation of atomic data for vapour shielding and of the models that use this data through comparison of simulation results with plasma gun, laser ablation and electron beam experiments.

Benchmark line radiation transport codes, including EIRENE, with a suitable set of simulation parameters using analytical models (where possible) and/or existing specialized codes.

Compare and understand the differences between dielectronic recombination rates predicted by different CR codes and assess the resulting impact on vapour shielding models.

Intended Outcomes

Data produced, evaluated and/or recommended in the CRP will be used to interpret data on the effect of disruptions and other extreme heat load events in present fusion plasma experiments.

Data produced, evaluated and/or recommended in the CRP will be used for modelling the effect of extreme heat load events in ITER and in other future fusion devices, and to help assess the viability of Li and/or Sn as a divertor material capable of continuous vapor shielding.

In addition, data produced, evaluated and/or recommended in the CRP will be used to simulate pellet ablation in present and future fusion devices.

Planned Outputs

A meeting report in the INDC (Nuclear Data Section) series will be produced after each Research Coordination Meeting.

Scientific articles will be produced by participants in the CRP.

The Knowledge Base and other web pages of the IAEA A+M Data Unit will be kept up-to-date to reflect the work of the CRP.

ALADDIN and other databases of the A+M Data Unit will be augmented with data produced or evaluated in the CRP.

If the data assembled merit it, a database of surface chemistry / sputtering / evaporation processes for relevant materials will be constructed and hosted at the A+M Data Unit.

A final report of the CRP will be published in a scientific journal.

Schedule of Activities

Q3 2018: Identification of participants, assembly of the CRP.

Q1 2019: First RCM.

Q2 2020: Second RCM.

Q3 2020: Mid-term review of the CRP.

Q4 2021: Third RCM.

2022: Development and publication of CRP final report.

Appendix V: Selected Recent Articles and Conference Contributions on Vapour Shielding in Fusion Devices

This Appendix contains a summary of relevant journal literature and contributions at major fusion energy meetings.

Journal literature

Vapour shielding for specific fusion wall materials

B. T. Brown, R. D. Smirnov and S. I. Krasheninnikov: "On vapor shielding of dust grains of iron, molybdenum, and tungsten in fusion plasmas," Phys. Plasmas 21 (2014) 024501. Online:

http://dx.doi.org/10.1063/1.4866599.

R. J. Goldston, A. Hakim, G.W. Hammett, M.A. Jaworski, J. Schwartz. "Recent advances towards a lithium vapor box divertor", Nuclear Materials and Energy 12 (2017) 1118. Online:

https://doi.org/10.1016/j.nme.2017.03.020

Sizyuk, Tatyana, and Ahmed Hassanein. "Scaling mechanisms of vapour/plasma shielding from laser-produced plasmas to magnetic fusion regimes." Nuclear Fusion 54, no. 2 (2014): 023004. Online:

http://dx.doi.org/10.1088/0029-5515/54/2/023004. (Development of simplified models.)

Sakuma, I., Y. Kikuchi, Y. Kitagawa, Y. Asai, K. Onishi, N. Fukumoto, and M. Nagata. "Experimental investigation of vapor shielding effects induced by ELM-like pulsed plasma loads using the double plasma gun device." Journal of Nuclear Materials 463 (2015): 233-236. Online:

http://dx.doi.org/10.1016/j.jnucmat.2014.10.020.

Skovorodin, D. I., A. A. Pshenov, A. S. Arakcheev, E. A. Eksaeva, E. D. Marenkov, and S. I. Krasheninnikov. "Vapor shielding models and the energy absorbed by divertor targets during transient events." Physics of Plasmas (1994-present) 23, no. 2 (2016): 022501. Online:

http://dx.doi.org/10.1063/1.4939537. (Presents different simplified models of vapour shielding.)

van Eden, G. G., T. W. Morgan, D. U. B. Aussems, M. A. van den Berg, K. Bystrov, and M. C. M. van de Sanden. "Self-Regulated Plasma Heat Flux Mitigation Due to Liquid Sn Vapor Shielding." Physical Review Letters 116, no. 13 (2016): 135002. Online:

http://dx.doi.org/10.1103/PhysRevLett.116.135002.

Kikuchi, Y., I. Sakuma, Y. Asai, K. Onishi, W. Isono, T. Nakazono, M. Nakane, N. Fukumoto, and M. Nagata. "Vapor shielding effects on energy transfer from plasma-gun generated ELM-like transient loads to material surfaces." Physica Scripta 2016, no. T167 (2016): 014065. Online:

http://dx.doi.org/10.1088/0031-8949/T167/1/014065.

Pestchanyi, Sergey, Richard Pitts, and Michael Lehnen. "Simulation of divertor targets shielding during transients in ITER." Fusion Engineering and Design 109 (2016): 141-145. Online:

https://doi.org/10.1016/j.fusengdes.2016.02.105.

Poznyak, I. M., D. A. Toporkov, S. V. Karelov, V. M. Safronov, and N. I. Arkhipov. "Properties of tungsten vapor plasma formed at conditions relevant to transient events in ITER at plasma gun facility MK-200UG." In AIP Conference Proceedings, vol. 1771, no. 1, p. 060006. AIP Publishing, 2016. Online:

https://doi.org/10.1063/1.4964214.

Eden, G. G., V. Kvon, M. C. M. Sanden, and T. W. Morgan. "Oscillatory vapour shielding of liquid metal walls in nuclear fusion devices." Nature communications 8, no. 1 (2017): 192. Online:

https://doi.org/10.1038/s41467-017-00288-y.

Pestchanyi, S., R. A. Pitts, and V. Safronov. "Validation of TOKES vapor shield simulations against experiments in the 2MK-200 facility." Fusion Engineering and Design 124 (2017): 401-404. Online:

https://doi.org/10.1016/j.fusengdes.2017.02.048.

Ibano, K., D. Nishijima, J. H. Yu, M. J. Baldwin, R. P. Doerner, T. Takizuka, H. T. Lee, and Y. Ueda. "Observation and particle simulation of vaporized W, Mo, and Be in PISCES-B plasma for vapor-shielding studies." Nuclear Materials and Energy 12 (2017): 278-282. Online:

https://doi.org/10.1016/j.nme.2017.01.016.

Vapour shielding for pellet ablation

Review article. B. Pégourié: “Review: Pellet injection experiments and modelling,” Plasma Phys. Control. Fusion 49 (2007) R87–R160. Online:

http://dx.doi.org/10.1088/0741-3335/49/8/R01.

Vapour shielding, generic or hard to classify

AlMousa, Nouf, and Mohamed A. Bourham. “Vapor Shield Models for Fusion Reactors Plasma-Facing Components.” Journal of Fusion Energy 35, no. 5 (2016): 786-794. Online:

http://dx.doi.org/10.1007%2Fs10894-016-0106-x.

Esmond, Micah, and Leigh Winfrey. "Radiation Heat Transfer and Vapor Shielding in a Two-Dimensional Model of an Electrothermal Plasma Source." Journal of Fusion Energy 35, no. 4 (2016): 643-651. Online:

https://doi.org/10.1007/s10894-016-0089-7.

Coburn, Jonathan, and Mohamed Bourham. "Ablation Simulation of Tungsten-Alternative Plasma-Facing Components due to Edge Localized Modes and Hard Disruptions." Fusion Science and Technology 72, no. 4 (2017): 692-698. Online:

https://doi.org/10.1080/15361055.2017.1352426.

Gebhart, T. E., L. R. Baylor, J. Rapp, and A. L. Winfrey. "Characterization of an electrothermal plasma source for fusion transient simulations." Journal of Applied Physics 123, no. 3 (2018): 033301. Online:

https://doi.org/10.1063/1.4998593.

Atomic processes, CR modelling

R. Ishizaki, P. B. Parks, N. Nakajima and M. Okamoto: “Two-dimensional simulation of pellet ablation with atomic processes,” Phys. Plasmas 11 (2004) 4064. Online:

http://dx.doi.org/10.1063/1.1769376.

D. Kh. Morozov, V. I. Gervids, I. Yu. Senichenkov, I. Yu. Veselova, V. A. Rozhansky and R. Schneider: “Ionization–recombination processes and ablation cloud structure for a carbon pellet,” Nucl. Fusion 44 (2004) 252. Online:

http://dx.doi.org/10.1088/0029-5515/44/2/005.

M Goto, S Morita and M Koubiti: “Spectroscopic study of a carbon pellet ablation cloud,” J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 144023. Online:

http://dx.doi.org/10.1088/0953-4075/43/14/144023.

22nd International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2016), Rome, 2016

Invited and oral contributions

Yusuke Kikuchi: Plasma-vapor mixed layer formation and its effects on energy transfer processes from ELM-like pulsed plasma heat loads to tungsten materials.

Poster contributions

P1.109 R. J. Goldston, Princeton Plasma Physics Laboratory (PPPL), NJ, USA: Recent Advances towards a Lithium Vapor Box Divertor.

P3.106 M. Iafrati: Modeling of lithium vapour cloud observed on FTU.

16th International Conference on Plasma Facing Materials and Components for Fusion Applications (PFMC 2017), 2017

Invited and contributed talks

None.

Poster contributions

P1-36 A. Kasatov, Budker Institute of Nuclear Physic and Novosibirsk State University, Russia: Experimental investigation of the process of tungsten ablation under the ITER-scale transient heat load.

18th International Conference on Fusion Reactor Materials (ICFRM 2017), Aomori, Japan, 5-10 November 2017

Plenary, invited and other talks

None.

Poster contributions

9PT34 N. Klimov, Troitsk Institute for Innovation and Fusion Research, Russia: Experimental Study of Vapour Shielding Effect on the Fusion Reactor Materials under Plasma Heat Loads Relevant to ITER Transient Plasma Events.

23rd International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2018), Princeton, NJ

Invited and oral contributions

None.

Poster contributions

Kenzo Ibano: Suppression of wall erosion by vapor shielding at low-Z and high-Z walls.

Jacob Schwartz: A lithium vapor box divertor similarity experiment for a linear plasma device.

Other conferences (no systematic search)

Kenzo Ibano (Osaka University): Particle simulation of plasma heat-flux dissipation by evaporated wall materials. Poster at 26th IAEA Fusion Energy Conference, Kyoto, Japan, 17–22 October 2016.

K. Ibano (Osaka University): Energy Dissipation by Vapor Shielding during Transient Loads. Presented at Fusion Energy System Studies (FESS) USA/Japan Workshop, NIFS, Toki-city, 27-29 March 2017.

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