Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology

Hosted by the Government of the Republic of Korea through the National Fusion Research Institute, Daejeon, Korea, 15-19 December 2014

Book of Abstracts

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Schedule

Monday 15 December 2014

08:30 - 09:00 Bas Braams, IAEA, and Jung-Sik Yoon, NFRI: Welcome.

09:00 - 09:30 David Campbell, ITER, Cadarache, France: Progress towards fusion energy at ITER.

09:30 - 10:00 Keeman Kim, NFRI, Daejeon, Korea: Design Concept of Korean Fusion Demonstration Reactor.

10:00 - 10:30 *Break.*

10:30 - 11:00 Robin Barnsley, ITER, Cadarache, France: Overview of progress with ITER spectroscopic systems.

11:00 - 11:30 Valery A. Kurnaev, MEPhI, Moscow, Russian Federation: Survey of plasma-material interaction and atomic data studies for fusion in Russia.

11:30 - 12:00 Jonathan Tennyson, UCL, London, United Kingdom: Electron-molecule collision data using the R-matrix method.

12:00 - 14:00 *Lunch.*

14:00 - 14:30 Annarita Laricchiuta, CNR IMIP, Bari, Italy: Thermodynamics and transport properties of high-density hydrogen plasma.

14:30 - 15:00 Gregor Karwasz, N. Copernicus University, Torun, Poland: Known and unknown in electron-atom and molecule scattering.

15:00 - 15:30 Viatcheslav Kokoouline, UCF, USA: Uncertainty evaluation in theoretical calculations of cross sections and rate coefficients.

15:30 - 16:00 *Break.*

16:00 - 16:30 Shinichiro Kado, Kyoto University, Japan: Excited state temperature of atomic helium in MAP-II steady-state linear divertor simulator.

16:30 - 17:00 Dmitry Fursa: Electron scattering from the molecular hydrogen ion and heavy particle collisions with atoms and molecules.

18:00 - 20:00 *Welcome reception.*

Tuesday 16 December 2014

08:30 - 09:00 Kerry Lawson, CCFE, Culham, United Kingdom: applications of atomic data to JET spectroscopic measurements.

09:00 - 09:30 Tomohide Nakano, JAEA, Naka, Japan: Experimental evaluation of W recombination and ionization rates/cross-sections.

09:30 - 10:00 Sebastijan Brezinsek, Forschungszentrum Jülich, Germany: Atomic and molecular spectroscopy in the scrape-off layer of high temperature fusion plasmas.

10:00 - 10:30 *Break.*

10:30 - 11:00 Pascal Quinet, University of Mons,Belgium: Atomic structure and radiative data calculations for heavy elements of interest in fusion plasma research. Theoretical challenges and recent advances.

11:00 - 11:30 Martin O'Mullane, University of Strathclyde,United Kingdom: Atomic data provision in the ITER era - an ADAS perspective.

11:30 - 12:00 Roger Hutton, Fudan University, China: Atomic structure and spectroscopy of highly charged tungsten ions and relevance to ITER diagnostics.

12:00 - 14:00 *Lunch.*

14:00 - 14:30 Yuri Ralchenko, NIST, Gaithersburg, USA: Atomic spectroscopic data and spectra modeling for highly-charged high-Z ions.

14:30 - 15:00 Izumi Murakami, NIFS, Toki, Japan: NIFS atomic and molecular database and spectroscopic modelling for fusion plasma.

15:00 - 15:30 Ursel Fantz, IPP Garching and University of Augsburg, Germany: Relevance of molecules in ionizing and reombining plasmas in the divertor and in negative ion sources for fusion.

15:30 - 16:00 *Break.*

16:00 - 18:00 Poster Session.

Wednesday 17 December 2014

08:30 - 09:00 Olga V. Ogorodnikova, MEPhI, Moscow, Russian Federation: Comparison of deuterium trapping in ion- and neutron-damaged tungsten-based materials: experiments and modelling.

09:00 - 09:30 Howard Scott, LLNL, Livermore, CA, USA: atomic physics and radiation transport in inertial confinement fusion simulations.

09:30 - 10:00 Yannick Marandet, Aix-Marseille University, France: On the influence of turbulent fluctuations on atomic and plasma-material interaction data for edge plasma modelling.

10:00 - 10:30 *Break.*

10:30 - 11:00 Detlev Reiter, Forschungszentrum Jülich,Germany: Atomic, molecular and PMI databases in the B2-EIRENE family of 2D edge plasma transport codes.

11:00 - 12:00 All: Discussion on atomic and molecular data.

12:30 - *Free afternoon.*

Thursday 18 December 2014

08:30 - 09:00 Shigeru Morita, NIFS, Toki, Japan: Recent progress on tungsten spectroscopy and its data analysis in Large Helical Device.

09:00 - 09:30 Christian Linsmeier, Forschungszentrum Jülich, Germany: The first wall of fusion reactors: A challenge for materials research.

09:30 - 10:00 Marek Rubel, KTH, Stockholm, Sweden: Material migration in JET with metal plasma-facing components: impact on fuel inventory and modification of diagnostics mirrors.

10:00 - 10:30 *Break.*

10:30 - 11:00 Guang-Hong Lu, Beihang University, Beijing, China: Hydrogen and helium behaviors in tungsten: new insights from modeling and simulation.

11:00 - 11:30 Takuji Oda, Seoul National University, Seoul, Korea: Development of potential model for tritium behavior in tungsten.

11:30 - 12:00 Igor E. Garkusha, IPP, Kharkov, Ukraine: Features of plasma interaction with tungsten brush surfaces under transient plasma loads simulating ITER divertor conditions.

12:00 - 14:00 *Lunch.*

14:00 - 14:30 Klaus Schmid, IPP Garching, Germany: Bridging the gap between atomic and molecular data and fusion experiments.

14:30 - 15:00 Heun-Tae Lee, Osaka University, Japan: Towards an improved understanding of hydrogen transport in tungsten.

15:00 - 15:30 Teppei Otsuka, Kyushu University, Japan: Retention and release behaviors of hydrogen in fusion reactor materials studied by means of tritium tracer techniques.

15:30 - 16:00 *Break.*

16:00 - 16:30 Predrag Krstic, Stony Brook University, NY,USA: Scientific challenges in the fusion plasma-material interface.

16:30 - 17:30 All: Discussion on plasma-material interaction data.

19:00 - 21:00 *Conference dinner*.

Friday 19 December 2014

08:30 - 09:00 Hyun-Kyung Chung, IAEA, Vienna, Austria: Past, present and future activities of IAEA Atomic and Molecular Data Unit.

09:00 - 09:30 Suk-Ho Hong, NFRI, Daejeon, Korea: Introduction to activities on IAEA dust database.

09:30 - 10:00 Bas Braams, IAEA, Vienna, Austria: Data evaluation and uncertainty estimates for calculated A+M data.

10:00 - 10:30 *Break.*

10:30 - 11:30 All: Reviews: Atomic, Molecular and Plasma Material Interaction Data.

11:30 - 12:00 All: Data needs: Plasma Modeling and Diagnostics.

12:00 - 12:30 All: Conclusions and Recommendation.

12:30 *Close of Meeting.*

Posters

(The poster session is Tuesday 16 December, 16:00-18:00.)

(P) K. M. Aggarwal and F. P. Keenan: Energy levels and radiative rates for Br-like ions with $z \leq 50$.

(P) G. Colonna: Self-consistent vibrational and electronic kinetics in a H_2/He plasma.

(P) Xiaobin Ding: Visible M1 transition of the ground state of W^{26+}- W^{28+} ions.

(P) Makoto Imai: Charge exchange collision cross sections for tungsten ions.

(P) Younggil Jin: Analysis of tungsten long-term retention and re-emission with ion-induced defect generation under ion oversaturation condition.

(P) Hyun-Su Kim: Possibility of underestimation on sputtering yield of graphite and tungsten pfcs.

(P) Duck-Hee Kwon: Theoretical electron-impact ionization cross sections of P-like ions, W^{17+}, and W^{+}.

(P)Thomas W. Morgan: Determination of absolute erosion yields and S/XB values via cavity ring-down spectroscopy in the Pilot-PSI linear device.

(P) K. Park, S. Y. Sim, W. Lee and C. H. Oh: Deuterium plasma diagnostics using collisional-radiative model including molecular effects.

(P) Ben Xu, Xiaoyang Wang, Yinan Wang and Wei Liu: The hydrogen's influence on core structure of dislocations in PFM tungsten.

(P) Yang Yang: Magnetic field sensitive spectroscopic lines and their prospects in atomic and astrophysics.

(P) Deqiong Zhu and Takuji Oda: Influence of hydrogen-vacancy interaction on the mobility of hydrogen and vacancy in bcc-metal.

Progress towards fusion energy at ITER

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Established by the signature of the ITER Agreement in November 2006 and sited at St Paul Lez Durance in southern France, the ITER project involves the European Union (including Switzerland), China, India, Japan, the Russian Federation, South Korea and the United States. ITER is a critical step in the development of fusion energy: its role is to confirm the feasibility of exploiting magnetic confinement fusion for the production of energy for peaceful purposes by providing an integrated demonstration of the physics and technology required for a fusion power plant.

At the core of the facility, the ITER tokamak will confine a plasma heated initially by particle beams and high frequency radio waves to temperatures in the region of 100 – 200 million K, at which point the deuterium-tritium fuel will react, producing up to 500 MW of fusion power. The primary aim of the project is to sustain such plasmas for periods of several hundred seconds with a fusion power gain, Q (ratio of thermal fusion power to injected heating power), of at least 10, while the ultimate goal is to demonstrate an essentially continuous mode of operation with $Q \geq 5$ which could be exploited in a fusion power plant producing electricity. Research activities will extend beyond the study of burning plasmas to the testing of key power plant technology: for example, the performance of tritium breeding modules, which are prototypical of the tritium breeding blankets forming a critical component of the fuel cycle in a fusion reactor, will be tested in ITER.

In the burning plasma regime, where internal heating due to fusion products dominates other (external) forms of heating, the physics of the interaction between the high energy α -particles produced by D-T fusion reactions and the thermal background plasma assumes a central role, and this will open new windows on the study of magnetically confined plasmas. In addition, the challenges of handling the high heat and particle fluxes generated by the plasma will need to be addressed successfully to sustain high fusion power production under quasi-stationary conditions. Key issues in these areas of fusion plasma research will be discussed and aspects of the ongoing supporting research in the international fusion programme will be highlighted. An overview of the operations plan leading to the demonstration of significant fusion power production and fusion power gain will also be presented.

The presentation will outline the physics basis for designing a device capable of producing several hundred MW of fusion power, describe the major elements of the research programme designed to demonstrate high fusion power gain in long duration plasmas at power levels of up to 500MW, discuss some of the key challenges in achieving and sustaining the required plasma conditions for high fusion power production, and summarize the present construction status of the project.

Design concept of Korean Fusion Demonstration Reactor

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Korean Fusion Energy Development Promotion Law (FEDPL) was enacted in 2007 to promote a long-term cooperative fusion research and development among participating industries, universities and research institutes. As a following step, a conceptual design study for a steady-state Korean fusion demonstration reactor (K-DEMO) has been initiated in 2012.

One special concept discussed of K-DEMO is a two-staged development plan. At first, K-DEMO is designed not only to demonstrate a net electricity generation ($Q_{eng} > 1$) and a self-sustained tritium cycle (Tritium breeding ratio, TBR > 1.05), but also to be used as a component test facility. Then, at

its second stage, a major upgrade is carried out by replacing in-vessel components in order to show a net electric generation on the order of 500 MWe. After the thorough 0-D system analysis, the major radius and minor radius are chosen to be 6.8 m and 2.1 m, respectively, considering practical engineering feasibilities. In order to minimize the deflection of wave and maximize the efficiency, a top launch high frequency (> 200 GHz) electron cyclotron current drive (ECCD) system is considered as one of the main candidates for the current profile control and off-axis current drive of K-DEMO. For matching the high frequency ECCD, a high magnetic field is required and it can be achieved by using high performance Nb_3Sn-based superconducting conductor currently being used in accelerator magnet area and the peak magnetic field is approaching to 16 T with the magnetic field at the plasma center above 7 T. Key features of the K-DEMO magnet system include the use of two toroidal field (TF) coil winding packs, each of a different conductor design, to reduce the construction cost and save the space for the magnet structure material. Also, the configuration is constrained by maintenance considerations, leading to a magnet arrangement with large TF coils, which minimize the magnetic ripple, and widely-spaced poloidal field (PF) coils to accommodate removal of in-vessel components as large modules. K-DEMO incorporates a vertical maintenance design. Pressurized water is the most prominent choice for the main coolant of K-DEMO when considering balance of plant development details. Considering the plasma performance and the peak heat flux in the divertor system, a double-null divertor system becomes the reference choice of K-DEMO.

A design concept and radial builds for K-DEMO considering a vertical maintenance scheme are presented together with preliminary design parameters.

Overview of progress with ITER spectroscopic systems

Robin Barnsley

ITER Organization, Cadarache, France

[The ITER spectroscopic systems serve for machine protection, basic control of plasmas, physics studies and advanced control. An overview is given of the diagnostic systems with attention to instrument requirements, impurity emission modeling and atomic data. –Eds.]

Survey of plasma-material interaction and atomic data studies for fusion in Russia

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A brief survey of activity on generation and application of atomic and molecular (A+M) and plasma-material interaction (PMI) data for fusion science and technology in Russia is given. This covers both the current and future project (ITER and beyond). This includes:

• PMI data generation for plasma facing components choice in fusion reactors;

• application of PMI databases to ITER design;

• PMI data needs;

• A+M data generation for integrated modeling of fusion experiments (transport, radiation losses, spectroscopic diagnostics),

• application of A+M databases and kinetic codes to tokamaks ITER and T-15 diagnostics,

• A+M data needs.

Electron-molecule collision data using the R-matrix method

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Electron collisions with molecules can provoke an number of processes including excitation (rotational, vibrational and electronic) and fragmentation of the molecule (both via electron attachment and directly) as well as, at higher collision energies, processes such as ionization. Detailed models of molecule-rich regions of fusion plasmas, such as in the divertor, require significant amounts of data on molecular processes. While experiments can yield some information on the processes listed above on stable molecules, they struggle to obtain results of any sort on open shell (radical) species, tritium-containing compounds or vibrationally hot molecules.

Quantum mechanical calculations, such as those using procedures offered by the R-matrix method [1], in principle provides a way of generating the necessary information. However theoretical calculations often show strong model dependence and, particularly in situations where they cannot be validated by experiment, it is hard to be specific about the underlying uncertainty in any predicted cross section or rate.

The talk will give examples of recent electron-molecule calculations performed using the R-matrix method for important plasma processes such as vibrational excitation and electron impact dissociation. It will explore some of the issues raised by these calculations and discuss the prospects for future, fusion-related studies.

[1] J. Tennyson, Electron - molecule collision calculations using the R-matrix method, Phys. Rep., 491, 29 (2010).

Thermodynamics and transport properties of high-density hydrogen plasma

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The development of new technologies and experimental techniques has triggered intensive theoretical research on the modeling of spatially confined quantum systems [1, 2] and also of extreme-high-pressure plasmas [3] like in stellar envelopes [4].

The thermodynamic properties and transport coefficients of non-ideal, high-density hydrogen plasma have been investigated, accounting for quantum effects due to the change in the energy spectrum of atomic hydrogen when the electron-proton interaction is considered embedded in the surrounding particles. High-density conditions have been simulated assuming atomic hydrogen subject to a screened Coulomb potential, to account for the surrounding plasma.

The ionization equilibrium is affected by the pressure ionization phenomenon, deeply investigated in literature as resulting from the non-ideal Debye-Hückel corrections [5]. The influence of the plasma leads to a correction term lowering the ionization potential, that corresponds to the so-called self-energy shift [5,6], $\Delta = -e^2/\lambda_D$, thus leading to an effective value Ieff = $I_0 - \Delta$, where I_0 is the ionization potential of the isolated, unperturbed hydrogen atom. Actually an additional lowering is due to the effect of the presence of a screened Debye potential on the eigenvalues for electronic levels obtained

solving the Schrödinger equation, correspondingly observed in the case of box confinement. Furthermore the ensemble of levels affects also the internal partition function of H atom in the Saha equation.

The effects of non-ideality in the thermodynamics of high-density hydrogen plasma on transport properties have been investigated in the frame of the Chapman-Enskog theory.The electrical conductivity of Debye plasma also exhibits a dependence on the total electron density that is affected by the pressure ionization, i.e. the minimum behavior of the conductivity and the *Mott transition* merging to the fully ionized regime.

[1] T. Sako, G. H. F. Diercksen, J. Phys. B 36 (2003) 1681.

[2] U. Merkt, J. Huser, M. Wagner, Phys. Rev. B 43 (1991) 7320.

[3] R. Dutt, A. Mukherjee, Y. P. Varshni, Phys. Lett. A 280 (2001) 318.

[4] D. G. Hummer, D. Mihalas, D., Astrophys. J. 331 (1988) 794.

[5] D. Kremp, M., Schlanges, W. D. Kraeft, *Quantum Statistic of Nonideal Plasmas*, in Springer Series on Atomic, Optical and Plasma Physics 25 Springer, 2005.

[6] M. Capitelli, G. Colonna, A. D'Angola, *Fundamental Aspects of Plasma Chemical Physics: Thermodynamics*, in Springer Series on Atomic, Optical, and Plasma Physics 66 Springer, 2012.

Known and unknown in electron-atom and molecule scattering

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The variety of atomic and molecular processes in fusion plasmas requires detailed knowledge and/or prediction of numerous cross sections, both for scattering on neutral as well on ionized species. A brief outline of the state of data from experiments, theories, semi-empirical methods and existing databases will be given. Our recent work on electron-CH_4 [1] will be used as an exemplary case.

The state of knowledge on cross sections will be classified according the level of certainty that can be ascribed to every process (and class of targets).

• Elastic cross sections are pretty well known for small targets, like CH_4 but experiments and theories lack and/or disagree on polar targets (including H_2O), and heavier targets (like C_6H_6).

• The level of agreement between elastic and momentum transfer cross sections is still poor for molecular targets. Re-analysis of existing swarm , cross-check of different modeling codes (two-term Boltzmann, multi-term, Monte Carlo) and new beam measurements at low energies are needed.

• Born approximation works pretty well for IR-active vibrational cross sections but not for Raman modes; various theories generally disagree, especially at resonances

• Rotational excitation, especially on polar molecules, could be also described by Born approximation, but even for water [2] the picture could be more complicated

• Ionization cross sections (integral and differential) cross sections can be described by Born-Bethe Binary Encounter Model (BEB), and agrees well with experiments as we analysed the case of series CH_4-CH_3F…-CF_4 [3]. That model operates only two parameters – the kinetic and potential energy of electrons at a given molecular orbital. However, we are not able to predict *partial* ionization cross sections: work is in progress.

• Electronic excitation cross sections present the biggest challenge: recent calculations [4] in CH4 agree with experiments on dissociation cross sections but direct electronic excitation measurements seem unreliable.

A tentative map of “white spots” in knowledge of cross sections for scattering on ions, radical and molecules in species relevant to fusion plasmas will be discussed.

[1] Mi-Yong Song et al., *J. Phys. Chem. Ref. Data*, to be submitted

[2] D. Field et al., Čurík et al.. *Phys. Rev. Lett.* 97 (2006) 123202

[3] G. P. Karwasz, P. Możejko, Mi-Young Song, *Int. J. Mass Spectrom.*, 365/366 (2014) 232

[4] W. J. Brigg, J. Tennyson and M. Plummer, *J. Phys. B* 47 (2014) 185203

Uncertainty evaluation in theoretical calculations of cross sections and rate coefficients

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In theoretical calculations of cross sections involving molecules, it is not yet a common practice to assess uncertainty of obtained results. The reason for it is the the multi-step nature of the most of theoretical calculations: For example, many scattering calculations rely on potential energy surfaces obtained in a different study, in which the uncertainty is not assessed. In such a situation, an independent uncertainty evaluation of final theoretical data becomes nearly impossible. On the other hand, if the uncertainty of each step in the theoretical treatment is assessed, then it is possible, at least in principle, to estimate the uncertainty of final theoretical data (cross sections and rate coefficients). We have adapted an approach developed in nuclear physics to the problem of uncertainty evaluation in theoretical determination of cross sections in two-body collisions, such as electron-molecule collisions. There are several advantages of the approach: (1) It allows one to evaluate the uncertainty of final theoretical cross sections, if uncertainties of all parameters used in the model are available. (2) It can deals with parameters of the theoretical model that are correlated. The correlation between parameters of the model reduces uncertainties of the final cross section. (3) If experimental data including uncertainties are available, the approach allows one to combine theoretical and experimental results using the Bayesian analysis. The last point is particularly important because it gives a standardized way to produce evaluated (recommended) cross sections, uncertainties, and, if needed, covariance matrices. The approach seems to be quite general and can be used for different AMO processes.

This work is partially supported by the National Science Foundation, Grant No PHY-10-68785 and by the NFRI Plasma Technology Research Center of Korea.

Excited state temperature of atomic helium in MAP-II steady-state linear divertor simulator

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Measuring the ion and/or neutral temperatures in divertor/edge plasmas or divertor-simulating low-temperature plasmas based on the *passive* optical emission spectroscopy is a challenging issue. In this regime, low-principal quantum number (*n*) states exhibit only the Doppler broadening, while the high-*n* states *can* exhibit both the Doppler and Stark broadenings if the electron density is relatively high.

Doppler-Stark spectrometry [1] for helium plasmas was applied to the MAP-II (material and plasma) steady-state linear divertor simulator at the University of Tokyo [2]. We have masured the line profile of several atomic helium spectra (He I), in which the contribution balance of Gaussian (Doppler component) and Lorentzian (Stark component) is different. In particular the transitions of 2^1S -3^1P

(501.567 nm), 2^1S -7^1P (335.455 nm), and 2^3P -7^3D (370.500 nm) were found to be useful in detecting the behavior of the excited state temperature [1].

We have pointed out that the ^1P states population is dominantly contributed from the ground state – reflecting the atomic temperature, due to the resonant transition and the radiation trapping processes. On the other hand, high-n ^3D states are dependent on the population flow between the states – reflecting the ion temperature for the recombining plasma while the heated excited level above Griem's boundary for the ionizing plasmas. This fact results in the thermal disequilibrium between the states [3]. These senarios were suppoted by the evaluation based on the collisional-radiative model for He I for which the electron temeprature and density were measured using a laser Thomson scattering [4] and/or a electrostatic probe.

In the detached plasma for helium discharge where the volumetric recombination dominates, the temperature of the electrons, ions and atoms became close to each other (~ 700 K), suggesting the achievement of the thermal equilibrium around the gas temperature. In the ionizing plasmas, on the other hand, the temperature of the excited states of the atomic helium was reveled to be dependent on the states. This disequilibrium feature became more apparent as the electron density n_e increases (1300 K ~ 20000 K for $n_e \sim 10^{13}$ cm^{-3}).

Acknowledgment: The data presented in this contribution were obtained when the author belonged to the University of Tokyo (~2013). MAP-II device has recently been moved to Tsukuba University.

[1] S. Kado Y. Iida, S. Kajita et.al., J. Plasma Fusion Res. 81, 810(2005).

[2] S. Kado, K. Suzuki, Y. Iida, and A. Muraki, J. Nucl. Matter. 415, S1174–S1177 (2011).

[3] S. Kado, presented at the PSI conference 2014 (Kanazawa, Japan) ; K. Suzuki, master thesis dissertation, the Univ. Tokyo (2010)[in Japanese].

[4] F. Scotti and S. Kado, J. Nucl. Matter. J. Nucl. Matter. 390-391, 303-306 (2009).

Electron scattering from the molecular hydrogen ion and heavy particle collisions with atoms and molecules

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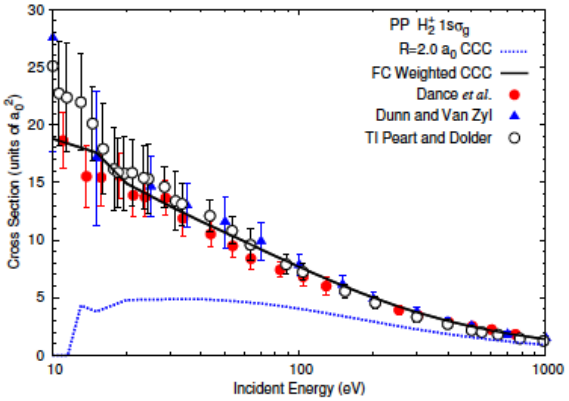
Electron collisions with the molecular hydrogen ion H_2^+ and it isotopologues (D_2^+, T_2^+, HD^+, HT^+ and DT^+) play an important role in determining the dynamics of fusion, astrophysical and laboratory produced low-temperature hydrogen plasmas. Experimentally H_2^+ is produced by electron-impact ionization of H_2. This can leave H_2^+ in one of its 20 bound vibrational states and many experimental measurements are taken with H_2^+ populated in a range of vibrational states.

Here we report the progress of implementing the adiabatic convergent-close-coupling (CCC) method in its application to electron scattering from vibrationally excited H_2^+ and its isotopologues. The present adiabatic CCC results are used to obtain electron scattering cross sections that are resolved for vibrationally excited states of H_2^+ and its isotopologues. Adiabatic cross sections were weighted according to vibrational population of the molecule and comparison with experiment is excellent across the energy range from near threshold to 1 keV. Account of the vibrational distribution of H_2^+ was found to be very important [1].



In the figure we present proton production cross sections calculated in the 351-state adiabatic CCC model. Cross sections for scattering from vibrationally excited states were weighted according to the Frank-Condon (FC) distribution. These results are compared with the present fixed-nuclei calculations at R = 2.0 a_0 and measurements of Peart and Dolder [2] Dunn and Van Zyl [3] and Dance *et al.* [4].

Recently we have extended the CCC method to heavy particles collisions with atoms and molecules within a semiclassical formulation. The CCC method has been applied to antiproton scattering from H_2 molecule [5] and noble gases. We are developing a formulation that takes into account charge exchange processes that will allow us to consider proton/ion collisions with atoms and molecules. Results for proton-hydrogen collisions will be presented at the meeting.

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Applications of atomic data to JET spectroscopic measurements

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An analysis of C IV emission from the JET divertor illustrates the atomic data requirements for the modelling of edge impurities in tokamaks. The analysis is applied to a database of 250 JET pulses, allowing T_e of the C IV emitting plasma region, T_e (C IV), to be determined. A clear dependence of T_e (C IV) on the bulk plasma n_e is found. The sensitivity of the analysis to the available R-matrix calculations of electron collisional excitation rates is discussed.

Electron collisional ionization from excited states is usually included in collisional-radiative models. It is found for the C III and C IV 'spectroscopic' levels (principal quantum number $n \leq 5$) that this mechanism is not significant, whereas ionization to excited levels is of greater importance, particualrly during impurity influxes into the plasma.

A need for calculations of accurate fast α-particle collisional excitation rates is identified. This would enable the significance of additional W radiation due to the excitation of W ions by fast α-particles

with subsequent radiation to be assessed and the sensitivity of a possible α-particle diagnostic using Kr line intensity ratios to be judged.

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Experimental evaluation of W recombination and Ionization rates/cross-sections

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It has been decided that ITER (International Thermonuclear Experimental Reactor) will be operated with tungsten (W) divertor from the day one because of low tritium retention property of W. However, due to high atomic number (=74), W ions tend to accumulate at the plasma core, and strong line radiation from the W ions reduces the plasma temperature. Thus, one of the issues in plasma operation with W divertor is to prevent W ions from penetrating plasmas towards the core, and therefore, it is important to measure the W density at the core quantitatively. To determine the W density from measured W spectral line intensity, various atomic data for W ions are needed; ionization and recombination rates are needed in order to calculate fractional abundance of W^{q+} ion (q: charge state), and photon emission coefficients, which are calculated with a collisional-radiative model, are needed to determine W^{q+} density from the measured intensity of a W^{q+} spectral line. Hence, uncertainty of the determined W density heavily depends on uncertainties of the atomic data in addition to uncertainty of the measurement. However, in most cases, calculated W atomic data without uncertainty evaluation are used in the analysis. Therefore, it is very difficult to mention the uncertainty of the determined W density. This motivates experimental evaluation of the calculated W atomic data.

This talk presents two experimental evaluations of the W atomic data: one is evaluation of a ratio of W^{44+} ionization rate over W^{45+} recombination rate performed in a thermal plasma of JT-60U tokamak. The other is evaluation of a ratio of W^{44+} ionization cross-section over W^{45+} recombination cross-section in a mono-energy plasma of Tokyo EBIT device. One of the advantages of this method is cancellation out of electron temperature/energy dependence of excitation rate/cross-section from 4s to 4p level, enabling direct conversion of an intensity ratio of W^{44+} 4s-4p spectral line over W^{45+} 4s-4p spectral line to a density ratio of W^{44+} over W^{45+} by using a coronal model, which can be compared to calculated W^{44+}/W^{45+} density ratio.

Comparison in the thermal plasma of JT-60U shows good agreement within 30%, indicating that the ratio of W^{44+} ionization over W^{45+} recombination rates calculated by FAC are evaluated to be accurate within 30%. In addition, comparison in the mono-energy plasma of Tokyo EBIT also shows good agreement except for some peaks due to resonant structures of dielectronic recombination. Reasons for this disagreement are not yet known. Finally, this talk makes a proposal for potential diagnostic lines in ITER: W^{62+} 3s-3p spectral line and W^{63+} 3s-3p spectral line together with a similar evaluation method to those described above for W^{44+} and W^{45+} 4s-4p spectral line.

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Atomic and molecular spectroscopy in the scrape-off layer of high temperature fusion plasmas

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[*]See Appendix: F. Romanelli et al., Proceedings of the 24th Fusion Energy Conference 2014, Saint Petersburg, Russia

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Atomic and molecular spectroscopy in the plasma edge of fusion plasmas gained importance in the last decade. Three principle categories can be distinguished here: (i) impurity spectroscopy to determine sputtering sources of s and extrinsic seeding species strength, (ii) hydrogen spectroscopy to determine the divertor characteristics and recycling fluxes, and (iii) extrinsic impurities used to probe the plasma in a non-pertubative way. Due to the high temperature of the magnetically confined edge plasma, even in the Scrape-Off-Layer, are dissociation and ionisation processes responsible for the destruction of atoms and molecules and only in detached divertor conditions can recombination become prominent. Electron impact excitation from the ground state and radiative decay are the basic processes though for a set of important atomic and molecular species in fusion plasmas (D, C, He) meanwhile collision-radiative models exist which take e.g. level mixing, metastable, cascades etc. into account. The situation is worse for W which is currently the most important impurity due to the first divertor selection in ITER and the abandon of carbon as plasma-facing material PFM.

We present the actual status in deuterium molecular spectroscopy used to determine the composition of the plasma-facing surface with respect to the atomic-to-molecular flux ratio as well as the isotopic composition of the recycling flux. The identification of T_2 and DT Fulcher-band spectroscopy from the JET Tritium Trace Campaign and the high sensitivity to determine the T content of about 0.1% will be shown. Secondly, the hydrocarbon catabolism had been studied extensively in TEXTOR by injection of all types of hydrocarbons $C_x(D,H)_y$ and the footprint of the injected species in the edge plasma measured. Inverse photon efficiencies for spectroscopic detectable molecules (CD, CD^+, C_2) and atoms/ions D, C, C^+, C^{2+} detected and compared with the HYDKIN code. Comparison of the ionic species with ADAS data revealed up to a factor 5 differences in the efficiency which is likely due to direct excitation in higher state and not the electronic ground state. Moreover, the sputtering yields of the newly selected PFMs in ITER: Be and W and associated experiments with the JET-ILW to determine the erosion yield and molecular destruction in the plasma will be presented. Thereby, chemical assisted physical sputtering (CAPS) in JET limited discharges has been identified to be responsible for a fraction of the total be source. The measurement of CAPS was performed via the A-X band of the Bed molecule in the SOL and simultaneous measurement of BeI and BeII whereas BeII includes both types of physical sputtering. Under constant bombardment of D^+ and high fuel content in the interaction layer (supersaturation) is the release mechanism strongly dependent on the surface temperature. The increase of the surface temperature from 570K to about 800K extinguished the channel for CAPS. About 1/3 of the total yield at impact energy of 75eV is caused by CAPS: its contribution rises at lower energies though still an energetic threshold exists. Finally, experiments with WF6 injection are presented which deliver S/XBs-values to calibrate WI photon fluxes from W limiters at TEXTOR and divertor plates at JET. The first documentation of swift chemical sputtering of W via WD is presented.

Atomic structure and radiative data calculations for heavy elements of interest in fusion plasma research. Theoretical challenges and recent advances

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In the present contribution, we discuss some recent advances concerning the determination of radiative parameters (transition probabilities, oscillator strengths, radiative lifetimes) in lowly ionized heavy atoms ($Z \geq 37$). Some emphasis is put on the procedures followed to obtain the new results but also on the difficulties associated with their experimental and theoretical determination.

Among the heavy elements considered, tungsten deserves a particular attention. Indeed, it is well known that spectroscopic parameters of W ions are essential for exploring the physical conditions in Tokamak plamas such as ITER in which tungsten is currently considered to be a primary candidate for the plasma-facing material in the divertor region. In fusion reactors, tungsten will be sputtered from the wall as a neutral element and the determination of the W influx rate to the core plasma will depend on a calculation of transport from the wall surface through the srape-off layer. Consequently, the identification of emission lines and the knowledge of radiative parameters from all ionization stages of tungsten will greatly aid modelling of the plasma edge and scrape-off layer transport and facilitate the analysis of net tungsten influx rates. In this context, the new sets of atomic data obtained in our work for the first ionization stages of tungsten will be extremely useful for future fusion plasma analyses.

Atomic data provision in the ITER era - an ADAS perspective

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[The presentation describes the Atomic Data and Analysis System database, computer codes and collaborative organization and its use in ITER's Integrated Modelling and Analysis Suite. –Eds.]

Atomic structure and spectroscopy of highly charged tungsten ions and relevance to ITER diagnostics

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Due to a number of favorable physical and chemical properties, Tungsten is strongly considered as a plasma facing material for the ITER fusion device. Some of the properties of Tungsten leading to this consideration are: high energy threshold of sputtering, low sputtering yield, high re-deposition efficiency, low tritium retention, and excellent thermal properties. However, even though the sputtering properties are favorable, some Tungsten atoms and ions will still make their way into the fusion plasma. Tungsten, being a high Z element, will contribute to a large fraction of energy being radiated out of the plasma and lead to plasma cooling, this can be quite drastic if too many tungsten ions enter the plasma.

To control the Tungsten influx, first good quality atomic structure data of many charge states of Tungsten ions are needed to examine spectral regions where the influx and transport can be monitored. The charge state distribution of Tungsten ions in the plasma is a good indication of the amount of power that will be radiated out. There are models predicting the charge state distribution of tungsten ions in a fusion plasma however, we argue in this paper that these models may lack some important contributions concerning ionization from metastable levels and hence produce inaccurate results. Our hypothesis is based on a large amount of spectroscopic work done at the Shanghai electron beam ion trap laboratory on visible spectroscopy of tungsten ions in the charge states ranging from W^{13+} to W^{28+}.

We have also investigated the soft x ray spectral region for tungsten ions expected to exist in the divertor region. It is interesting to note that only 108 lines from all charge states of tungsten have been reported in the wavelength region of 200 – 400 Å.This is important as the ITER soft x ray spectrometer will operate in this wavelength region. Even more interesting is that only five of these lines come from charge states other than W6+ and the identification of four of these can be questioned. We have investigated the soft x ray spectra of W^{11+}-W^{15+} and identified a number of lines/spectral features in the region 200 – 400 Å.

Atomic spectroscopic data and spectra modeling for highly-charged high-Z Ions

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Since tungsten is currently accepted as the plasma-facing material for ITER divertor, its spectroscopic characteristics in different ionization stages from neutral to 60-70-times ionized are being actively studied in various laboratories. In addition, examination of spectra from other high-Z elements may help establish isoelectronic trends that serve as an important test for tungsten spectroscopy. In this talk we will present an overview of the research program on spectroscopy of tungsten and other heavy elements carried out at the National Institute of Standards and Technology (NIST).

The Atomic Spectra Database (ASD) at NIST presently contains a significant amount of evaluated spectroscopic data for all elements up to Z_N=110 although substantial gaps in data coverage still exist. The current status of ASD and other atomic and plasma databases at NIST will be presented in detail. On the experimental side, the NIST Electron Beam Ion Trap (EBIT) is actively used to generate x-ray and extreme ultraviolet spectra from high-Z ions with charges of Z=35-65. The analysis of the measured spectra and identifications of new spectral lines from such elements as W, Hf, Ta, Pt, Au are assisted by a large-scale collisional-radiative (CR) modeling of non-Maxwellian EBIT plasma. Then, CR modeling is extended to Maxwellian fusion plasmas to determine feasibility of the measured lines for plasma diagnostics in tokamaks, stellarators, and other plasma devices. The efficiency of precision spectroscopy on EBITs will be exemplified by the measurements of inner-shell LMN dielectronic satellites in W ions with an open 3d shell. Their analysis requires development of an anisotropic CR model based on magnetic sublevels for autoionizing states. We will also briefly describe an ongoing effort on validation and verification of CR models for heavy elements within the framework of the Non-LTE Code Comparison Workshops.

NIFS atomic and molecular database and spectroscopic modelling for fusion plasma

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We have constructed atomic and molecular (AM) databases on collision cross sections and rate coefficients and make them available via the internet at http://dbshino.nifs.ac.jp/ since 1997. Data compilation was started in the 1970s at the Institute of Plasma Physics (IPPJ), Nagoya University by a working group. The first compilation on atomic data of H and He and their isotopes for fusion research was published as a IPPJ report [1], since then we have compiled AM data on collision processes and plasma-wall interactions for fusion plasma research. Currently our database system has AMDIS (cross sections and rate coefficients of electron collision processes for atomis; 675,439 records as of Sep. 22, 2014), CHART (cross sections of heavy particle collision processes for atoms; 7,054 records), AMDIS-MOL and CHART-MOL (collision cross sections and rate coefficients for

molecules; 3,951 records), SPUTY (sputtering yields for solids; 2,084 records), and BACKS (backscattering coefficients of solid surface; 396 records). The databases are retrievable and numerical data are shown as a graph or a table. Each data record contains bibliographic information, so original publications are traceable. We also provide many satellite databases which provide data files on, for example, electron dissociation attachment to molecular hydrogen, published as a NIFS-DATA report [2]. Our work on AM data evaluation for some ions are published as IPPJ-AM reports and NIFS-DATA reports.

We also work on spectroscopic modelling on impurity elements for fusion plasmas. Carbon and iron ions are studied for long time as main impurities. Atomic data and spectroscopic modelling on Fe ions are also important for astrophysical plasmas and we validated Fe XVII atomic data and modelling using Large Helical Device (LHD) [3]. Recently we intensively work on tungsten modelling and spectroscopic measurements with LHD and compact electron beam ion trap device (CoBIT). Our tungsten modelling can reproduce measured extreme ultravaiolt spectra at 1.5-7 nm with W^{20+}-W^{36+} ions. Their emission peaks of principal quantum number n=5-4 transitions at 1.5-4 nm are useful to examine charge state distributions of tungsten ions for plasma with electron temparture less than 2 keV [4].

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Relevance of molecules in ionizing and recombining plasmas in the divertor and in negative ion sources for fusion

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The plasma edge of fusion devices is characterised by cold temperatures with respect to the hot core. Specifically in the divertor region the electron temperature is typically a few eV; in the detached plasma regime where volume recombination dominates it is even below one eV. Here, the survival length of hydrogen molecules produced at surfaces by recombination of hydrogen particles is high. These molecules can undergo a variety of reactions, among them dissociation, dissociative ionization and dissociative recombination. The relevance of these reactions depends on the plasma regime, i.e. whether the plasma is ionizing or recombining or in the transition between both regimes. Another important parameter is the vibrational and rotational excitation in the ground state of the molecule and the ion, which in particular depends on the isotope.

Molecules are also important in the negative hydrogen ion sources under development for the neutral beam heating systems for ITER. In the low temperature plasma of these sources the degree of dissociation is less than one and vibrationally excited hydrogen molecules play a dominant role in the plasma chemistry. In particular they are important for the production of negative hydrogen ions in the plasma volume. In these sources, the plasma is separated by a magnetic filter field into an ionizing and a recombining part and dissociative recombination of molecular ions becomes important in the transition region. Close to the extraction system exists an ion-ion plasma (i.e. positive and negative ions are dominant whereas electrons play a minor role) and mutual neutralization with molecular ions is a dominant process. Molecules are also involved in the beam neutralisation and important for beam

spectroscopy. Since these sources operate in hydrogen and in deuterium isotope effects are of particular interest.

In addition, the presence of molecular species in the plasma may influence the interpretation of diagnostic results. An example is the Balmer line radiation, which is sensitive on dissociative excitation and dissociative recombination and has consequences on the determination of the recycling flux. As a consequence, collisional radiative models need to be used in which the different species are coupled to the excited states of the hydrogen atom: molecules, molecular ions, the atom itself and its ion, and negative ions. The realization however, relies strongly on the availability of the underlying cross sections, which should be taken into account preferably vibrationally – and even more demanding rotationally – resolved. In particular here, the low energy range from the threshold to a few tens of eV is relevant. In contrast, the high energy range of several keV is of interest for beam characterisation.

Comparison of deuterium trapping in ion- and neutron-damaged tungsten-based materials: experiments and modelling

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Tungsten is a reference material for the high-flux, low-ion-energy region of the divertor in ITER and a candidate plasma-facing material for DEMO. Those plasma-facing and structural components of fusion reactors will be exposed to 14 MeV neutrons (n) together with high rate of helium (He) and hydrogen (H) production due to transmutation reactions. Additionally, plasma-facing materials will be irradiated with the hydrogen fuel (T and D) and helium (He) with low energies. Experimental data on the influence of displacement damage on hydrogen accumulation, recycling and permeation in materials are very scarce, and the detailed theoretical understand of hydrogen transport through damaged materials is incomplete. These data are strongly required not only for ITER, but also for future fusion power reactors such as DEMO.

In the present contribution, experimental investigation of radiation-induced defects produced in W by irradiation with energetic self-ions was done via decoration with deuterium [1] and compared with the data for neutron-irradiated W in HFIR reported in [2]. The experimental data of the deuterium concentration at radiation-induced defects created by irradiation with 20 MeV W ions and with HFIR neutrons at room temperature show a reasonably good agreement at least up to 0.3 dpa. For the first time the coefficient of similarity was found experimentally to be ~0.65 ± 0.02 and ~0.85 ± 0.05 from direct comparison of deuterium concentration at radiation-induced defects produced by self-ions and neutrons after D plasma exposure at 470 and 700-773 K, respectively.

The experimental study was accompanied by theoretical investigation. The theoretical coefficient of similarity between neutrons in HFIR and 20 MeV W ions was estimated to be K_{sim}=0.34 using the classical approach. The theoretical value of K_{sim}=0.34 is about two times less than the experimental value of K_{exp}=0.65 obtained in the case of deuterium decoration of both kinds of radiation-induced defects with low and high de-trapping energies for deuterium. It means that high energy PKAs can play more important role in production of similar damage structure by irradiation with self-ions and neutrons which is responsible for deuterium retention. The model assuming that all cascades with an energy higher than T=150 keV split into identical sub-cascades gives value of $K_{sim}=0.64 \pm 0.01$ for coefficient of similarity between HFIR-neutron and 20 MeV self-ion irradiations in agreement with experimental value of $K_{exp}=0.65 \pm 0.01$. Consequently, splitting of high-energy part of cascades might take place in W and be sufficient in formation of radiation damage structure.

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Atomic physics and radiation transport in inertial confinement fusion simulations

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The pursuit of inertial confinement fusion depends heavily on simulations to understand the interplay of a myriad of physical processes. Radiation transport is a key physical process, serving as an important energy transport mechanism and providing crucial diagnostic information. The radiation transport in turn both depends on and affects the atomic physics. When local thermodynamic equilibrium (LTE) applies, the primary material information required is the opacity, depending mainly on atomic structure and material temperature, with the temperature strongly influenced by the radiation transport. When LTE does not apply, transitions dependent on the radiation field more directly affect the computation of opacities and emissivities, significantly complicating simulations. In both cases, radiation transport introduces a non-local aspect to the interaction between the material and the radiation field that must be incorporated into simulations.

This presentation focuses on computational methods for simulating radiation transport, with an emphasis on the interactions between radiation and matter. We give an overview of widely used approaches for transporting photons. We then discuss coupled systems, describing the microphysics of the interactions between radiation and matter and how these interactions impact methods for handling the non-local aspects. Examples will be drawn primarily from simulations of experiments on the National Ignition Facility (NIF) but will extend to tokamak edge plasmas.

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On the influence of turbulent fluctuations on atomic and plasma-material interaction data for edge plasma modeling

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Most of the current global edge modeling, and in particular the ITER divertor design effort hinges on transport codes such as SOLPS. These codes take as input a variety of atomic and molecular (AM) data as well as plasma material interaction (PMI) data. A consistent derivation of transport equations from the Braginskii equations imposes to smooth out the fluctuations due to turbulence by an averaging procedure. This procedure provides a theoretical justification for anomalous cross-field transport terms [1], but should also be properly applied to sources related to atomic physics, as already clear from Ref. [1]. In practice, instead of being performed on the physical quantities present in the equations (e.g. ionization and recombination rate coefficients), the averaging is performed on the fluctuating quantities (n_e,T_e). In other words, the implicit assumption is that $\langle S(n_e,T_e)\rangle \approx S(\langle n_e\rangle,\langle T_e\rangle)$, where S comprises atomic data such as ionization and recombination rate coefficients, or sputtering yields. This can be a crude approximation because of the non-linear density and temperature dependences of such coefficients, as pointed out by several authors [2]. This issue could be especially relevant in the scrape-off layer (SOL), where the relative fluctuation levels can be of order unity. The same is true for plasma material interaction (PMI) data (e.g. sputtering yields), especially for main chamber recycling and erosion, since most of the PMI there results from plasma

filaments. If the mean plasma temperature is below the sputtering threshold, one would conclude that sputtering is essentially supressed, while positive temperature fluctuations could in practice result in much higher impurity influxes.

We have thus undertaken to quantify the resulting modeling uncertainties at the level of transport equations. Our goal is to obtain properly defined effective, "fluctuation-dressed", AM&PMI data for transport codes and possibly also for diagnostic interpretation (when dealing with time averaged signals). We focus here on impurity generation and transport (Be and W), and assess the effects of fluctuations using both turbulence code results and stochastic models. Neutral impurities penetration is shown to be favored by density fluctuations, which can increase local densities by up to an order of magnitude. Properly accounting for temperature fluctuations on AM source terms is shown to shift the ionization balance towards lower temperatures, changing abundances by factors of up to 5. Overall, the effects of fluctuations on impurity transport are shown to become substantial for dense SOLs (several 10^{19} m^{-3}). The derivation of effective rate coefficients capturing these effects is presented.

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Atomic, molecular and PMI database in the B2-EIRENE family of 2D edge plasma transport codes

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Magnetic fusion edge plasma transport codes resort to a large number of atomic, molecular and PMI data, in order to quantify the related processes in the context of plasma flows in the outer and near target of the fusion plasma. Many different edge plasma codes are in use, common to most of them is a 2D or 3D CFD treatment of the main plasma (electrons, ions) components, and a kinetic (often Monte Carlo) treatment of the atomic, molecular and some low concentration impurity ions. The B2-EIRENE family of codes is such an example. It builds, e.g., the transport part also of the SOLPS suit of codes, notably the SOLPS_ITER code hosted by ITER-IO.

These primary computational tools, which take A+M+PMI data as input, have to deal with the much more involved 'plasma state of matter' issues first. They are far less mature and limited in their predictive quality as compared to computational tools in other areas of sciences, e.g. to those taking nuclear data as input.

The data challenge (A+M+PMI data) in codes such as B2-EIRENE (see: www.eirene.de) often comes in at a peripheral level, dealing with albeit important, sometimes decisive, sub-components of the model. Computational fusion plasma science, at least with so called integrated models covering many individual effects in a single model, can be regarded as an attempt to separate, computationally, known from unknown. This is needed in order to isolate the latter sub-components and make them accessible for experimental quantification. If this separation is made, A+M data fall into the category 'known', plasma turbulence and flows and all its consequences fall in the category 'unknown'.

In the present contribution we publicly expose the status of atomic, molecular and PMI data in fusion edge plasma codes, and we discuss their journey from the raw, unprocessed data towards condensed, properly averaged data used in codes, as well as first attempts to quantify the uncertainty propagation during this data processing step. This latter is achieved by a (linear) sensitivity analysis option build into collision radiative codes for fusion plasma transport applications (as available under: www.hydkin.de) .

Recent progress on tungsten spectroscopy and its data analysis in Large Helical Device

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A comprehensive study of tungsten spectra has been started from 2010 experimental campaign in Large Helical Device. The tungsten spectra have been observed by injecting tungsten pellet [1] in three wavelength ranges of visible, VUV and EUV ranges. In the visible range a magnetic forbidden dipole transition from highly ionized tungsten ions was observed for the first time in fusion devices [2]. A huge number of tungsten spectra have been also measured in the visible (3000-7000Å) [3] and VUV (300-3000Å) [4] ranges when the spectrometer directly observes a tungsten pellet ablation cloud with extremely low temperature (<10eV) and high density (~10^{18}cm^{-3}).

In the EUV (10-500Å) range the tungsten spectra have been observed not only the wavelength spectrum but also radial profiles in the plasma core. The observed tungsten spectra in the EUV range are identified and analyzed the spectra using HULLAC code. The radial profile of tungsten spectra is quantitatively analyzed for W^{44+} and W^{45+} ions and those density in plasmas is estimated assuming a pratical ionization balance at measured electron temperature profile. The observed tungsten ionization stage is compared with a result from the impurity transport code calculation [5]. A big difference is observed between the measured and calculated tungsten ionization stages. In order to determine practical ionization and recombination rates, which are really necessary for the tungsten transport study in fusion plasmas, the radial profile has been observed for many ionization stages of tungsten ions at wide electron temperature range, i.e., $0.1 \leq T_e \leq 2.0$keV. Some of them are comapred with impurity transport results. The ionization balance of tungsten ions is discussed in the coference with newly observed problems in tungsten spectroscopic study [6].

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The first wall of fusion reactors: A challenge for materials research

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The operating conditions in DEMO and a fusion power plant will add a number of new aspects to the list of requirements for plasma-facing materials. Other than for current fusion experiments and even ITER, the high neutron dose changes material properties with respect to mechanical properties (embrittlement) and composition (transmutation). Efficient energy production requires high coolant temperatures, calling for material and component solutions with sufficient high-temperature strength. The operation with D-T and the breeding of tritium require solutions against continuous tritium losses into structural materials and cooling media. Finally, a fusion power device must demonstrate passive safety properties in case of off-normal operational events, e.g. loss of coolant. Currently available materials for the first wall and divertor components of fusion devices fail in one or more of these criteria. In addition, essentially no data for first wall materials is available which allows predictions of erosion and hydrogen isotope retention due to plasma exposure after extended neutron exposure.

In this presentation several material solutions for the issues mentioned above will be discussed. In recent years, a number of advanced material concepts have been developed in order to address DEMO and power plant requirements. In particular, composite materials, smart tungsten alloys and hydrogen isotope permeation barriers are investigated. The status of these material developments will be summarized and future research needs, in particular also with respect to plasma-material interaction experiments with neutron-irradiated materials, are identified.

Material migration in JET with metal plasma-facing components: impact on fuel inventory and modification of diagnostics mirrors

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Since August 2011 the JET tokamak has been operated with the ITER-Like Wall (JET-ILW): beryllium (Be) in the main chamber and tungsten (W) in the divertor. i.e. the material configuration recently decided for ITER. Material erosion and fuel inventory studies are among top priorities of the JET-ILW programme. Various types of diagnostic tools, i.e. marker tiles and wall probes including test mirrors, have been employed to assess the overall material migration pattern. The specific goals of this work were to determine: (i) fuel retention in the divertor; (ii) erosion-deposition pattern of

beryllium and other species; (iii) the reflectivity and surface morphology of mirrors studied within the First Mirror Test at JET for ITER.

Analyses of in-vessel components have shown the erosion of Be inner wall limiters and the deposition of material on the upper tiles in the inner divertor leg. The thickest deposits, up to 15 □m, contain mainly beryllium with some minority species: carbon and also nitrogen from edge cooling. Their content is low: Be/C concentration ratio >16; Be/N >45. Also fuel inventory in JET-ILW is small, both relative: Be/D >10 in deposits and absolute being below $5x10^{18}$ cm^{-2}. This value is distinctly lower than in JET with carbon walls (JET-C) where layers of a few hundreds of micrometers were formed. The study has not identified on wall components the formation of flaking deposits which could contribute to the dust formation. It should also be stressed that the reflectivity of polycrystalline molybdenum mirrors tested on the main chamber wall was retained or even improved in some cases. This result may have a positive impact (e.g. cost reduction) on the planning and development of maintenance procedures for ITER diagnostic mirrors. The options will be presented. These findings indicate advantages of metal components in comparison to the carbon surrounding.

Hydrogen and helium behaviors in tungsten: New insights from modeling and simulation

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Tungsten is considered to be one of most promising condidates for the plasma-facing materials in next-step fusion reactors, for which hydrogen (and isotopes) and helium retention and blistering remains a key issue that needs to be addressed. Via modeling and simulation, we have investigated the behaviors of hydrogen and helium as well as their synergy in tungsten [Nucl Fusion 54, 086001 (2014)], which is found to be more complicated and interesting than we have known before.

For hydrogen, a generic microscopic vacancy trapping mechanism for hydrogen bubble formation in tungsten is revealed in terms of optimal charge density [Phy Rev B 79, 172103 (2009)], which can be also applied to a grain boudary [Nucl Fusion 50, 025106, (2010)]. The hydrogen solubility is found to be always enhanced by anisotropic strain in tungsten, independent of the sign of strain, which suggests a cascading effect of hydrogen bubble growth in tungsten [Phy Rev Lett 109, 135502 (2012)]. The critical hydrogen concentration for the hydrogen bubble formation in tungsten is predicted using the thermodynamic model in combinatin with the first principles [J Phys: Condens Matt 26, 395402 (2014)].

The relative stability of helium at different interstitial sites is shown to scale quantitatively with the effective volume of helium, as defined by the helium-induced lattice stresses. Empirically, the effective volume of helium can be approximated by the hard-sphere lattice model, but not by the commonly used point-lattice model [Europhys Lett 96, 66001 (2011)]. Further, the “electrophobic” interaction provides a leading mechanism responsible for the experimentally observed phenomenon of helium self-trapping in metals.

Helium is shown to exhibit a strong attraction with hydrogen in tungsten [Nucl Fusion 50, 115010 (2010)], which can lead to a preferential accumulation of hydrogen surrounding helium in the near-surface region, thus blocking the hydrogen permeation into deeper bulk. On the other hand, hydrogen molecule cannot be formed in a helium-vacancy complex due to the occupancy of helium at the vacancy center, suggesting that helium can miligate the formation of hydrogen and thus bubbles in tungsten, consistent with the exprimental observation.

More insights can be further expected to understand the hydrogen and helium behaviors in tungsten, which will contribute greatly to resist the plasma irradiation in the fusion reactor.

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Development of potential model for tritium behavior in tungsten

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Tritium accumulation in plasma facing components such as tungsten is considered as an important fusion engineering issue, because (1) it affects the feasibility and economy of tritium fuel cycle and (2) the accumulation amount is vital information to make a plasma operation scenario that meets a radiation-safety regulation limit. Therefore, experimental data on the tritium accumulation has been largely acquired in the last decade. In order to predict the tritium accumulation in a fusion environment using those experimental data, it is needed to fill gaps between fusion reactor conditions and experimental conditions in tritium flux, neutron flux and fluence, etc, based on detailed understanding of the tritium behavior. Computational simulations in an atomic scale are expected to contribute to revealing the tritium behavior.

Among several available computational methodologies, classical molecular dynamics (MD) method has an advantage in its low computational cost. MD can deal with millions of atoms, and thus can simulate complex defects, such as ones composed by multiple vacancies and multiple tritium atoms. The low computational cost is realized by describing interatomic interactions with simplified model functions, so-called potential model. Due to this simplification, however, the accuracy of simulation results depends on the quality of potential model. For tungsten-tritium systems, two potential models [1, 2] have been widely utilized in MD simulations. However, their descriptions of tritium-vacancy interaction are not necessarily satisfactory, which motivates us to develop a new potential model.

This research aims to develop a new tungsten-hydrogen potential model which can adequately reproduce a great number of ab-initio calculation results on energy and force. The model function is composed by multiple basis functions [3] and their coefficients are uniquely determined by solving linear simultaneous equations. First, a two-body potential model for magnesium oxide is constructed to verify the methodology. The constructed potential model gives good agreement with ab-initio calculation on energy and force. Good performance is also confirmed in MD simulations on the melting point, the thermal expansion behavior, and the radial distribution functions. Next, the methodology is extended to include many body interactions using a form of the embedded atom model. By this extension, the agreement with ab-initio calculation on energy and force is largely improved. A comprehensive assessment with respect to tritium-vacancy interaction energies in tungsten will be given in comparison with the two existing potential models and ab-initio calculation.

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Features of plasma interaction with tungsten brush surfaces under transient plasma loads simulating ITER divertor conditions

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Castellated configuration of the divertor targets allows mitigation of the currents on the surface and minimization of the stresses that cause pronounced cracking of tungsten surface under the high heat loads from the intense transient events such as disruptions and ELMs in ITER. Nevertheless, castellated edges of macro-brush armor elements can be a dominating source of the molten/solid dust particles which are injected into the surrounding plasma. Therefore, specific features of the edges erosion for castellated targets need to be comprehensively studied both in corresponding simulation experiments and with predictive numerical simulation.

Experimental simulations of ITER transient events with relevant surface heat load parameters (energy density up to 2.4 MJ/m^2 and the pulse duration of 0.25 ms) as well as particle loads (varied in wide range from 10^{23} ion/m^2 s to 10^{27} ion/m^2 s) were carried out with a quasi-stationary plasma accelerator QSPA Kh-50. Particular attention was paid to elaboration of damage of tungsten as a main candidate material for ITER divertor surfaces and also as prospective material for DEMO design.

The targets that combined in brush-like geometry were irradiated under different inclination angles. Surface analysis of the targets exposed to QSPA plasma streams, with measurements of the erosion patterns in the course of increasing number of plasma pulses has been performed. The mountain of molten material appears on the edge of castellated targets. Calorimetrical measurements have shown than heat load to the gaps surfaces on the depth of 5 mm inside was 2 time less than to frontal surface. The onset of dust particles ejection from the exposed castellated targets has been studied. Formation of resolidified bridges through the gaps of brush-like targets due to the melt motion is studied in dynamics. With following plasma impacts such resolidified bridges became additional source of W dust. The dust particles were injected both up and down plasma stream. The maximal velocity achieved 24 m/s.

Differences in evolution of tungsten substructure after exposures with helium and hydrogen plasma streams of different duration are analyzed.

Experimental results have been compared with performed numerical simulation with the MEMOS-3D code which has been adopted for the castellated geometry.

Bridging the gap between atomic and molecular data and fusion experiments

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The plasma in the scrape off layer of a magnetic confinement fusion plasma is defined by the power and particle flux from the confined core plasma and by the recycling of hydrogen species and generation of impurities at the location where its open field lines intersect with plasma-facing wall components. Both the recycling of the hydrogenic fuel species and the generation of impurities depend on surface processes: The balance of implantation vs. effusion of hydrogenic species from the wall during the recycling process is determined by diffusion and trapping of hydrogen in metallic first-wall components. The erosion of elements from the first wall is determined by physical or chemical sputtering by the incident particle flux. All of these processes also depend on the surface state (e.g. composition) which varies as material is eroded and subsequently re-deposited forming mixed-material layers.

Thus to describe the evolution of the first wall a coupled, self-consistent description of the particle sources at the surface and the migration of impurities in the plasma is required. To that end the WallDYN [1] code was developed. The code maintains a strict global material balance of all eroded and (re)deposited material and allows the tracking of the chain of subsequent erosion/re-deposition/re-erosion and re-deposition steps that define where material is finally net-deposited or net-

eroded. WallDYN couples state-of-the-art models for the surface processes (e.g. erosion, reflection, sublimation) with material redistribution data from trace-impurity plasma transport models in a fully self-consistent simulation.

The transport of hydrogen in metals is comonly described by diffusion trapping models. They are limited to traps with single de-trapping energies and a saturation occupancy of one. While they are successful in predicting typical mono isotopic ion implantation and thermal degassing experiments, they fail at describing recent experiments on isotope exchange at low temperatures. Therefore, a new modified diffusion-trapping model [2] with fill-level-dependent de-trapping energies that can also explain these new isotope exchange experiments was developed. It allows to test DFT predictions on the trapping energy as function of fill level against experiments by bridging the gap in length and time scale.

This presentation will demonstrate how WallDYN can be used to interpret recent results on fuel retention and layer deposition in JET and how the concept of fill-level-dependent trapping affects the picture of hydrogen retention in metals such as tungsten under loading by different isotopes.

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Towards an improved understanding of hydrogen transport in tungsten

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Tritium inventory and permeation will certainly grow more in importance with ITER and next step devices employing metal plasma facing materials or components, as a consequence of the expanded use of tritium coupled with longer pulse or steady state operation. Specifically, tungsten is presently planned for use in the ITER divertor and possibly as an armour material for the first wall in next-step devices.

To improve our modeling and predictive capabilities of tritium inventory and permeation in fusion devices employing tungsten, we must solve the hydrogen transport equation, which requires solution to the diffusion equation with appropriate boundary conditions and trapping parameters. In general, the boundary conditions and trap parameters are time dependent due to the physico-chemical changes occurring at the tungsten surface from material mixing / erosion processes or changes in bulk material properties from neutron or heat loads. Presently, large uncertainties exist in accurately determining the nature of such boundary conditions and trap parameters, which hinders a robust and accurate estimate of tritium inventory and permeation in fusion devices.

In this presentation, we present our on-going efforts to establish the foundation necessary to quantitatively predict hydrogen transport (release, trapping, permeation) in tungsten. We address the following three phenomena that are important for quantifying tritium transport. First, the changes in boundary condition and its impact on the inward diffusive flux as function of temperature due to impurity induced near surface changes (C, N, He, Ar, Ne) or by surface melting are discussed. Second, we present our effort on determining the fundamental parameter of hydrogen diffusion coefficient in the temperature range of interest in fusion ($300 < T < 1000$ K). Third, we present novel ion and electron beam experiments that appear promising in determining some of the fundamental helium or irradiation induced trap parameters, which may allow testing and bridging of first principle simulations with laboratory experiments.

Retention and release behaviors of hydrogen in fusion reactor materials by means of tritium tracer techniques

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Recently, we have established tritium (T) tracer techniques to visualize depth profiles of hydrogen (H) loaded into fusion reactor materials by gas absorption and ion/plasma implantation. Wide dynamic range of T detection up to 5 digits makes detailed depth profiling possible in comparison with conventional H detection in solid. Observing changes of the depth profiles by annealing and/or during storage after the hydrogen loading, H release mechanism and behaviors of H (diffusion and trapping) in the F82H steel and pure tungsten (W) were investigated.

It was found that the depth profiles of loaded H were composed of four components in depth as follows;

1) H in surface adsorbates: Any materials surfaces adsorb H atoms and its compounds like water and hydrocarbon molecules. Although some of H in the surface adsorbates is easily replaced with loaded T by isotopic exchange reactions, their behavior was hardly correlated with that of the loaded H. Instead, a T amount retained in the surface adsorbates significantly changed during the storage after the loading by the isotopic exchange with H in ubiquitous water molecules and moisture in surrounding atmosphere.

2) H in intrinsically modified surface layers: Separate from the surface adsorbates, surfaces of metals are easily oxidized as often appears as protective or passive oxide layers or coverage of some other precipitates (like carbides, sulfides, nitride and their mixtures) with thickness of a few tens nm. Mechanical works make any surfaces defective. Some of the loaded H was found to be retained in the modified surface layers probably by making OT, CT bonds and/or defects-assisted trapping. Because of large binding energy or trapping energy, H retained in the modified layers hardly moved at room temperature. But their effect on release of the loaded H in further deeper region was not clear. It should be noted that distinction of H in the modified surface layers from H in the adsorbates is quite hard but the T tracer technique enabled us to distinguish them.

3) H in defects/impurities induced by H loading behind the modified surface layers: H is trapped at defects or damages and segregated impurities induced by energetic H loading in the damaged region. This region was saturated by H trapping in the defects (probably stabilized by self-trapping) during the H loading. In the case of pure W, the thickness of this region anomalously increased by continuous H loading. Since the amount of trapped H in this region was very large, most of the previous investigations on behaviors of ion/plasma-implanted H in pure W have simply observed the trapped H in the damaged region.

4) H in far deeper region: H penetrated in the deeper region by diffusion. Most of H was in solution but some could be trapped at intrinsic defects such as dislocations and grain boundaries. Observing time sequences of the depth profiles in the deeper region, reliable bulk H diffusion coefficients were determined both for the F82H steel and pure W.

Scientific challenges in the fusion plasma-material interface

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Plasma-Material Interface (PMI) mixes materials of two worlds, creating in between a new entity, a P-M dynamical surface, which communicates between the two creating one of the most challenging areas of multidisciplinary science, which has many fundamental processes and synergies.

The traditional trial-and-error approach to PMI for future fusion devices by successively refitting the walls of toroidal plasma devices with different materials and component designs is becoming prohibitively slow and costly. Since erosion, sputtering, retention, redeposition, reflection, displacement, etc. originate from atomic processes at nanoscale we need to construct the PMI science from the bottom up, using atomistic approaches, recognizing its multi-scale character and building from the shortest, atomic, to the longest time and spatial scales.

I will consider the questions common for various PMI environments:

- Why is PMI of high importance for the controlled nuclear fusion?
- Why is it so difficult problem?
- How to build an effective scientific approach to study PMI, recognizing its multiscale character?
- How to validate theory with the plasma-facing surface experiments?
- How could be PMI processes in giga machines compared with atomistic results?
- What is the role of quantum mechanics and role of chemistry?
- What are the bounds of uncretainty of the PMI data?
- How to build an integrated theoretical-experimental approach?
- How to build an intergated and self-consistent PMI-plasma approach?

The answers will be discussed on examples of deffects creation, hydrogen retention and fuzz appearance in tungsten; on the role of lithium and oxygen in reduction of the hydrogen recycling; on chemical sputtering of carbon.

*Also collabrating with Princeton Plasma Physics Laboratory and Oak Ridge National Laboratory.

Past, present and future activities of IAEA Atomic and Molecular Data Unit

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The Atomic and Molecular Data Unit within the Nuclear Data Section of the International Atomic Energy Agency was formed in 1977 in order to review progress and achievements of atomic, molecular and plasma surface interaction data for the world-wide Fusion programme and stimulate international cooperation in measurement, compilation and evaluation of those data. Over the years the Unit has organized coordinated research projects, maintained databases and online codes and published reports, bulletins and books.

Activities over the 12 years since the previous broad meeting on atomic, molecular and plasma-material interaction data for fusion (Jülich, 2002) will be reviewed along with the vision for the Unit's activities in the next decade. The Unit plans to emphasize the uncertainty assessment and evaluation of currently available atomic and molecular data. In accordance with the development of the fusion program, much effort will be invested in the international coordination of the production and compilation of plasma-material interaction data relevant to DEMO or a fusion nuclear science facility.

Introduction to activities on IAEA dust database

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For the next step fusion device like International Thermonuclear Experimental Reactor (ITER), in-vessel dust particles will become very important issues: Dust production and accumulation inside the vacuum vessel may lead serious safety and operational issues by "radioactive" tritiated co-deposits of nano- to micrometer size which is the main source of mobilizable dusts in tokamaks as long as carbon-based PFCs are concerned. Melting and splashing of metal PFCs such as Be or W will cause different problems. Furthermore, amount of dust on hot surfaces in ITER is limited to 6 kg due to a strong chemical reactivity with air and stream (ITER accidental scenario). Furthermore, some of them have very high impact velocity up to several km/s which can easily damage the first wall or diagnostics.

For these reasons, it is essentially important to monitor in-vessel dusts where they are created, when they are created, and how much dusts are created, what are their physical dimensions, shape, and chemical composition. IAEA AMD unit has launched to investigate those issues, especially the size, shape, and chemical composition of in-vessel dusts through a Coordinated Research Project (CRP) "Characterization of Size, Composition and Origins of Dust in Fusion Devices". After three years of CRP, it has been decided that a dust database should be built to support in-vessel dust study. The database include machine configuration, campaign data, and dust database together. In this paper, we introduce the IAEA dust database developed in NFRI.

Data evaluation and uncertainty estimates for calculated A+M data

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It is a big challenge to develop methods for estimating uncertainties of calculated atomic and molecular data that do not require huge additional computational effort. The present contribution concerns the Unified Monte Carlo (UMC) approach [1,2] that is well established in the nuclear data community. UMC employs a Bayesian formalism:

$$p(\sigma) = C \times L(y_E, V_E \mid \sigma) \times p_0(\sigma \mid \sigma_C, V_C)$$

$$p_0(\sigma \mid \sigma_C, V_C) \sim \exp\{-(\tfrac{1}{2})[(\sigma-\sigma_C)^T \bullet (V_C)^{-1} \bullet (\sigma-\sigma_C)]\}$$

$$L(y_E, V_E \mid \sigma) \sim \exp\{-(\tfrac{1}{2})[(y-y_E)^T \bullet (V_E)^{-1} \bullet (y-y_E)]\},\ y=f(\sigma)$$

Here p_0 is a prior and p a posterior probability, L is a likelihood function for experimental data, y_E and V_E are measured quantities and their uncertainty matrix while σ_C and V_C are model parameters and their uncertainty matrix; function f implements the model. Metropolis (Markov chain) sampling is used to sample model parameters σ from the probability p and then to obtain the quantities of interest and their estimated uncertainties including correlations. Note that this is very different than fitting a best estimate for the parameter vector σ.

We discuss a possible application to the provision of uncertainties and their correlation structure for rovibrational molecular spectroscopy. Two key tools are taken for granted: a method to develop fitted potential energy surfaces (PES), for example [3], and a method to solve the nuclear Schrödinger

equation [4]. The PES is taken as the model prior and then the solution of the nuclear Schrödinger equation together with some accurate measured lines supply the posterior.

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Energy levels and radiative rates for Br-like ions with Z ≤ 50

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Atomic data for energy levels and radiative rates (A- values) are required for the modelling of a variety of plasmas, including fusion. With the developing ITER project the demand for such atomic data has considerably increased. For some elements, such as Fe, Ni and W, atomic data are available for many of their ions. However for other elements, such as Mo and Sn, similar data are either not available or are limited to a few levels/transitions. Much less attention has so far been devoted to Br-like ions. Therefore, in a recent paper Singh et al [1] have reported A- values for the electric dipole (E1) transitions for five Br-like ions, namely Sr IV, Y V, Zr VI, Nb VII and Mo VIII, i.e. with $38 \leq Z \leq 42$. However, they have listed energies only for the lowest 31 levels of the $4s^24p^5$, $4s^24p^44d$ and $4s4p^6$ configurations, and A- values only from the ground state $4s^24p^5\ ^2P^o_{3/2,1/2}$ to higher lying levels. These limited data are insufficient for detailed plasma modelling. Furthermore, for the calculations they included limited CI (configuration interaction) whereas it is very important for Br-like ions, as has already been clearly demonstrated for another ion, namely W XL [2]. More importantly, their reported results for energy levels as well as A- values cannot be reproduced, as has recently been discussed and demonstrated by us [3].

Therefore, apart from including a considerably larger CI, we extended the range of both levels and transitions, although in [3] only limited results were presented. In this work we extend the range of ions, i.e. with $43 \leq Z \leq 50$, or specifically Tc IX, Ru X, Rh XI, Pd XII, Ag XIII, Cd XIV, In XV, and Sn XVI. As earlier, we have adopted the General-purpose Relativistic Atomic Structure Package (GRASP) code, and for the calculations extensive CI among 39 configurations has been considered. The specific configurations included are: $4s^24p^5$, $4s^24p^44d/4f$, $4s4p^6$, $4p^64d/4f$, $4s4p^54d/4f$, $4s^24p^34d^2/4f^2/4d4f$, $4s^24p^24d^3$, $4s^24p4d^4$, $4s^24p^24d^24f$, $4s4p^34d^3$, $4p^54d^2$, $3d^94s^24p^54d/4f$, $3d^94s^24p^6$, $4s4p^55\ell$, $4p^65\ell$, $4s^24p^45\ell$, and $3d^94s^24p^55\ell$. These configurations have been carefully chosen, because of their interacting energy ranges, although other configurations, such as $3p^53d^{10}4s^24p^6$, $3p^53d^{10}4s^24p^54d$ and $3p^53d^{10}4s^24p^54f$, have also been tested, but have been excluded from the calculations because they generate levels at much higher energy ranges, and hence their impact on the lower energy levels is insignificant. Additionally, apart from the E1 transitions, we have also calculated A- values for the electric quadrupole (E2), magnetic dipole (M1) and magnetic quadrupole (M2) transitions, because for a complete plasma model their results are also desirable and their availability improves the accuracy of the calculated lifetimes (τ). Detailed results will be shown and discussed during the meeting.

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Self-consistent vibrational and electronic kinetics in a H_2/He plasma

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Recently we have developed a comprehensive state-to-state kinetic model, coupling selfconsistently the master equations for internal distribution of atomic and molecular species, the Boltzmann equation for free electrons in two-term approximation and the transport equation for photons using the ray-tracing approach. This kinetic model can be coupled with fluid dynamic equations to investigate high enthalpy flows in shock tubes and nozzle expansion, in 1D configuration [1] or can be solved using time dependent approach in local approximation. The model can also include electric and magnetic field in affecting flow properties and electron energy distributions.

The model features up-to-date set of cross sections for electron impact processes, rate coefficients for heavy particles collisions and radiative transitions, resolved over the internal excited states of the different atomic and molecular species [2]. This model has been used to study the H_2/He plasma formed during hypersonic entry in Jupiter atmosphere. The STS approach provides the most detailed level of description, fully considering the effect of nonequilibrium internal and electron distribution on the chemical rate coefficients. The results have shown the importance of radiation, resulting in non-local effects due to photons emitted in hot regions and reabsorbed when the plasma is cooling down. The effects are reflected on the electron energy distribution functions through superelastic collisions, which transfer energy from excited states to electrons, resulting in non-maxwellian distributions.

In this work we report recent results obtained applying the STS model to high-enthalpy supersonic nozzle expansion and gas-discharge conditions. In the first case, the chemical kinetics is dominated by atom-atom recombination process, resulting in non-Boltzmann H_2 vibrational distributions and also non-equilibrium atomic distributions formed by the electronion recombination process. It is also shown that the radiation model has a strong impact on the evolution of the distributions and internal temperatures along the nozzle axis, resulting in completely different atomic state distributions and electron energy distribution functions in the optically thin and thick cases [3]. Under low-pressure discharge conditions the kinetics is essentially dominated by electron impact and attachment processes. In particular, under low E/N conditions the kinetic energy gained by electrons from the electric field is mostly spent in pumping the vibrational distribution, which promotes chemical processes activated by the vibrational energy.

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Visible M1 transition of the ground state of W^{26+}-W^{28+} ions

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Tungsten (W) is one of the major candidates for divertor or wall material in the next generation magnetic confinement fusion reactors due to its favorable properties. Tungsten atoms will be introduced into plasmas and they will act as impurity ions. Although the heavy ion impurities may cause a serious radiation power loss, their visible line emissions may still helpful for diagnostics of the core and edge plasmas owing to their low opacities [1]. Accurate atomic data of energy levels and transition properties relevant for such line emission are indispensable for the precise measurement of plasma properties. In the present work, we carry out an elaborate non-empirical theoretical calculation for the electronic structures and the M1 transition properties of W^{26+} to W^{28+} ions.

Multi-configuration Dirac-Fock (MCDF) method is a widely used ab-initio method to carry out a relativistic calculation for many electron atoms or ions. The effect of electron correlations can properly be evaluated by choosing a suitable set of basis which consists of the orbitals and excitations among those orbitals. We employ the GRASP code for our present calculation [2,3]. We have carried out an MCDF calculation for the ground state multiplets of W^{26+} and W^{27+} ions [4,5] and the first excited state of W^{28+} ions. The Breit interaction was estimated in low frequency limits and the vacuum polarization effect was evaluated by perturbation. In the framework of a restricted active space (RAS) on the MCDF procedure, the visible M1 transitions of W^{26+} to W^{28+} have been calculated. We have obtained a good agreement with experiment in Tokyo-EBIT[4] and Shanghai permanent magnet EBIT [5] . The disagreement of the theory with the experiment is only about 0.03eV, which is about 1% of the experimental transition energy.

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Charge exchange collision cross sections for tungsten ions

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One of the urgent technical issues in materializing larger fusion devices is a need for using heavier elements in plasma-facing components. Tungsten element is attracting particular interests these days because of its specific aspects of high melting-point, good thermo-mechanical properties, low tritium retention, low sputtering rates, and so on. Since tungsten causes a serious problem of radiation power-loss brought by its high atomic number, charge-state resolved transport phenomena of tungsten ions in fusion plasma have become notably important feature in larger fusion devices. Use of tungsten impurities for diagnostics is also an important issue to consider. To accomplish these issues, charge exchange collision (electron capture and loss) cross sections involving ions of tungsten become

essential in both low-energy, up to 20 keV for tungsten projectile ions, and high-energy regions, up to 1 MeV NBI hydrogen atoms colliding with tungsten ions at rest.

We have experimentally produced total electron capture cross sections for low-q heavy-ions Be^{q+}, B^{q+}, C^{q+}, Fe^{q+}, Ni^{q+}, and W^{q+} (q = 1,2) ions colliding with atomic and molecular gas targets of He, Ne, Ar, Kr, H_2, CH_4, C_2H_6, C_3H_8, CO, CO_2, and N_2 at collision energy between 4 and 25 keV in the Van de Graaff accelerator facility in Kyoto University. We have extensively derived scaling laws for single-electron-capture cross sections for these collision systems using ΔIP, *i.e.*, the first ionization potential of the target atom/molecule subtracted by that of the projectile ion after electron capture. There used to exist some scaling formulae predicting electron capture cross sections for high-q peojectile ions at low-energy limit, but no such scaling behaviour had never been introduced for low-q projectile ions at low-energy until ours. We are also performing charge exchange cross section production at high-energy for diagnostic purposes using the Tandem accelerator facility in Japan Atomic Energy Agency (JAEA.) To produce cross sections of electron loss and transfer process for 1 MeV NBI hydrogen beam by tungsten impurity ions, cross sections of an equivalent electron capture process for 184 MeV (1 MeV/u) tungsten ions from atomic hydrogen target will be measured. In this measurement, ionization cross section of tungsten ions by NBI hydrogen beam will be obtained at the same time by analyzing the outgoing charge-states of the projectile tungsten ions. The target thickness is normalyzed using iron projectile ions, whose cross sections are well-resolved.

Analysis of tungsten long-term retention and re-emission with ion-induced defect generation under ion oversaturation condition

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Much of researches have reached nearly consensus that the long-term retention can be increased by the ion-induced defect generation resulted from ion oversaturation at tungsten PFC sub-surface[1, 2]. The effect of ion dose and induced thermal energy on ion-induced defect generation near oversaturation zone has not been yet fully examined[1]. This research was conducted to clarify the effect of ion dose and additional thermal energy on both ion-induced defect generation at oversaturation boundary and long-term retention because the thermal energy can be loaded on PFC by ion irradiation itself. The ion irradiation was performed by ECR plasma system with the condition of ion flux of 3.1 x 10^{21} $m^{-2}s^{-1}$ and incident energy of 100 eV relevant to ITER divertor (10^{20}-10^{24} $m^{-2}s^{-1}$, 100 eV) [2]. The irradiation time was varied with 0.5-4 hours in order to investigate the dose effect. The thermal-load experiments were also carried out by thermal plasma torch with condition of 5 MW/m^2 to relevant ITER divertor. The deuterium inventory was measured by secondary ion mass spectrometry (SIMS) and thermal desorption spectroscopy (TDS) in order to analyze the depth profile of retained-D and binding state of D with ion-induced defect. It was observed that defect distribution expands to deeper region with deeper position of oversaturation boundary for high ion dose case, implying that the depth distribution ion-induced defect could be increased with increment of implanted particle number due to trap site (defect) saturation in oversaturation zone. The depth-profile of retained-D was dependent on both surface temperature and oversaturation depth according to different diffusion aspect, inferring that the re-emission of retained-D could be changed by the PFC operation temperature and accumulated ion dose. The additional thermal energy effect was revealed that the relaxation of oversaturation zone due to annealing effect, which result in dislocation removal in grain at high temperature. The experimental findings suggest that the long-term retention and re-emission flux can be transiently changed by the generation and elimination of ion-induced defect near oversaturation boundary due to effect of accumulated ion dose and additional thermal energy during long-term operation. The additional effect of high energy ion (3 keV) on ion-induced defect will be demonstrated by collaboration with Hokkaido University.

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Possibility of underestimation on sputtering yield of graphite and tungsten PFCs

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In general, sputtering yield models for graphite and tungsten plasma-facing components (PFCs) to estimate the PFC lifetime and impurity influx in fusion devices has been developed without the morphological changes of surface which are induced by the deuterium plasma interaction with the PFCs. Previous studies on the morphological change of PFCs have been reported such as conical tip formation on graphite [1] and blister formation on tungsten [2]. Since the sputtering yield is increased with the incidence angle of ion [3], it is worth to study the effect of morphological changes of PFCs on the sputtering yield. In this study, it is focused on the mechanism of morphological changes of the graphite and tungsten PFCs by the deuterium plasma interactions and, in addition, it is observed that the increment of sputtering yields. Experiments were carried out with electron cyclotron resonance deuterium plasma and DC biased tungsten and graphite targets for the simulation of fusion edge plasmas. Sputtering yield is monitored by using the measurement of weight loss. For the graphite PFC, the formation of carbon-deuterium bonds by chemical reaction interacts with the sheath electric field results in formation of the conical tips on the graphite. Conical tip formation on the graphite increases the sputtering yield due to increase of local angle of ion incidence and additional energy transfer from backscattered ion. With the consideration of the morphological change of graphite, the sputtering yield is increased about 100% from the estimation of Roth model assuming the plane surface [4]. For the tungsten PFC, deuterium ion irradiation generates the blister formation on the tungsten surface. If imagines the dome shaped blister, the sputtering is enhanced around the dome where the local angle of ion incidence is maximum. Notes that this side of dome is mechanically weaken due to plastic deformation during the blister formation of tungsten. The sputtering of blister edge may be enhanced due to morphological change and eventually top plate of blister is ejected and the small sized dusts can be generated. It results in the local increment of sputtering yield of tungsten PFC. Results suggest that the estimation of sputtering yield of PFCs interacted with the scrape-off layer (SOL) deuterium plasma requires the possibility of its enhancement due to the morphological changes of surface.

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Theoretical electron-impact ionization cross sections of P-like ions, W^{17+}, and W^{+}

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Recent EII calculations for Fe^{11+} by Dere [1], using the flexible atomic code (FAC) [2] based on a distorted wave (DW) approximation, show a discrepancy with the test storage ring (TSR) work [3]. The theory falls below the measurement near the 3p direct ionization threshold and lies above the

measurement at higher energies. We performed an improved FAC-DW calculation helping to resolve much of these discrepancies. In our calculation, we take into account the 3l → nl' (n=3-35) excitation-autoionization (EA) channels near the threshold and the 2l → nl' (n=3-10) EA channels at higher energies, along with their detailed branching ratios [4]. We have extended our EII calculations for Fe^{11+} to P-like ions from P to Zn^{15+} and the total EII Maxwellian rate coefficients for plasma modeling are provided [5]. Similar methods were applied for EII calculations of W^{17+} [6] and W^{+} [7].

The calculated total EII cross section including direct ionzation (DI) and EA for Fe^{11+} agrees well with recent experiment except for 2l → nl' EA. For this excitaion the calculated cross section is larger than the experiment. The calculated total EII cross section for W^{17+} agree with recent experiment but the calculated total EII cross section for W^{+} is about 25% larger than experiments. R-matrix calculations have been carried out for collisional excitation cross sections of Fe^{11+} and W^{+} ions by debugging and parallelizing R-matrix routines implemented in original FAC which have fatal segmentation fault errors for those complex system calculations and are programed for single processor. The collisional excitaion cross sections calculated by the R-matrix method will be presented and compared with our previous results by the DW method in detail.

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Determination of absolute erosion yields and S/XB values via Cavity Ring-Down Spectroscopy in the Pilot-PSI linear device

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The large heat exhaust expected in DEMO (estimated between 600-1000 MW [1]) produces extreme challenges for plasma facing components (PFCs) in accommodating and controlling the resultant high heat fluxes, and motivates investigating innovative materials for the divertor region. Liquid metals offer several potential advantages over a solid PFC, such as the ability to replenish the eroded surface, immunity to the effects of neutron embrittlement and the potential to act as a self-regulating source of radiating impurities to shield the surface from excess heat loads. As low melting point metals lithium, gallium and tin are the leading candidates but, especially for the latter two, atomic data is incomplete or non-existent in current databases orientated around fusion research.

One of the crucial questions in using any PFC is what its erosion flux into the plasma will be. Generally a standard technique for tokamak research is to determine this spectroscopically using inverse photon efficiencies (so-called S/XB values [2]) relating photon and particle fluxes. However, without calculations from collisional radiative models or determination experimentally of S/XB values this methodology remains unavailable for tin and gallium. At FOM DIFFER a Cavity Ring Down Spectroscopy (CRDS) system has been installed to determine absolutely the density of neutrals in the plasma eroded from a liquid tin target. The system can also be used in principle with other species with ground-excited transitions in the near UV and visible wavelengths, offering a new methodology for erosion measurements. This system has been connected to the Pilot-PSI linear device [3] a high flux low temperature linear plasma device which produces conditions which well replicate those expected in the ITER and DEMO divertors. In combination with optical emission spectroscopy

or filtered camera observations the CRDS system can be used to determine gross erosion yields and S/XB values for a variety of plasma densities and temperatures. This can therefore provide valuable information on surface erosion levels under divertor conditions as well as atomic data useful to plasma diagnosticians. Initial results from the implementation of the CRDS system in Pilot-PSI will be presented.

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Deuterium plasma diagnostics using collisional-radiative model including molecular effects

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In order to diagnose electron temperature (T_e) and electron density (n_e) of deuterium plasma, spectroscopic method (line intensity ratio) based on collisional-radiative method was selected.

CR-model based atomic process was configured and some molecular process of the dissociative excitation [1], mutual neutralization [2,3] and dissociative recombination [4] process for the very low temperature were included in the CR-model. Optical emission spectrum was measured by a monochromator (Czerny-Turner type, spectral resolution 0.313nm) and all of optical system including monochromator was calibrated with quartz halogen lamp. The transition lines of Balmer series (Balmer-α : n=3→n=2, 656.101 nm, Balmer-β : n=4→n=2, 486.000 nm, Balmer-γ : n=5→n=2, 433.928 nm) were selected to diagnose the T_e and n_e of deuterium plasma. The diagnosed results by line intensity ratio were compared with electric probe diagnosis.

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The hydrogen's influence on core structure of dislocations in PFM tungsten

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The nuclear quantum effect is considered in the study to find possible stable positions of hydrogen's around the screw/edge dislocation cores of tungsten. Their influences on the splitting of the dislocation cores are investigated by hybrid QM/MD calculation. And also the Peirls potential of the dislocation mobility are calculated by NEB methods. The existence of the hydrogen is also considered to be important when the dislocation piles up in the proximity of the grain boundaries.

Magnetic field sensitive spectroscopic lines and their prospects in atomic and astrophysics

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Magnetic fields play an important role in determining the properties of plasmas, for example, through driving the energetics and dynamics of enormous solar flares on the surface of the sun. They are also used to restrict huge plasma fluxes in man made fusion device like Tokamak. Measuring the structure of magnetic field in such plasmas is therefore extremely important and useful for understanding and plasma control. The problem is that there are always many inconvenience or limitations on measuring the magnetic field in high temperature plasmas with traditional methods like Zeeman splitting.

A new possible method of measuring magnetic fields in such plasmas based on magnetic field sensitive (MFS) spectroscopic lines is under development. The main principle is that external magnetic field will lead a mixture of near quantum states leading to unexpected transitions to occur, whose strength is depended on the external magnetic field. Measuring strengths of these spectroscopic lines will lead to much information about the local magnetic field structure.

The first measurement of magnetic field sensitive line $2p^5 3s\ ^3P_0$-$2p^6\ ^1S_0$ of Ne-like Ar ions was done at the Livermore EBIT and reported in 2003 [1] .We followed this study, and calculated and measured different MFS lines of different ions [2-3] and found many possibilities for application to Tokamak plasma magnetic field diagnostics.

Recently we have been working on a spectral line in a single charge state of Iron which shows extreme sensitivity to its surrounding magnetic field. Through continuing these studies we hope to be able to suggest a method for measuring magnetic fields in hot plasma such as solar flare. We expect to have more to report on this at the time of the meeting.

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Influence of hydrogen-vacancy interaction on the mobility of hydrogen and vacancy in bcc-metal

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The retention of tritium in plasma facing component is a key issue related to the safety and economics of fusion reactors. Understanding the interaction between hydrogen isotopes and irradiation defects is indispensable to evaluate the tritium inventory in plasma facing component. In the present work, the influence of hydrogen-vacancy interaction (H-V interaction) on the mobility of hydrogen and vacancy in bcc-metal is studied by molecular statics (MS) and molecular dynamics (MD) simulations. α-iron is chosen as the modeling material because (1) both α-iron and tungsten have bcc structures and similar characteristics to hydrogen and (2) more reliable potential models are available for α-iron regarding the interaction with hydrogen. In addition, as one of the constitutive component of structural

component, the study of hydrogen-vacancy interaction in α-iron itself attracts great interest. In simulations, a reported Fe-H potential model [1] of the embedded atom method (EAM) is employed. MS and MD simulations are conducted by using the LAMMPS code. The three-dimensional periodic boundary conditions (PBC) are imposed to a supercell in order to model a bcc-Fe crystal.

The diffusivities of hydrogen and vacancy in the systems with and without vacancy are evaluated and compared. It has been found that the mobility of hydrogen is clearly decreased due to the binding interaction between hydrogen and vacancy when they co-exist in α-iron bulk, and that the decrease trend is more significant at lower temperatures. On the other hand, the influence of H-V interaction on the mobility of vacancy depends on the configuration of vacancies. The mobility is decreased for the isolated vacancies, while it is increased for the vacancy cluster. No influence from the vacancy configuration on the mobility of hydrogen is observed.

Furthermore, the diffusivities of hydrogen in systems with varied H/V ratios (V1-H1, V1-H3, V1-H6, V1-H12, V8-H8) are checked. The results indicate that the diffusivity of hydrogen increases with the H/V ratio increasing. A simple model to evaluate the effective diffusivity of hydrogen (D_{eff}) in the system with vacancy co-existing is proposed by summating the diffusivity of hydrogen atoms that are trapped in vacancy (D_{trap}) and the diffusivity of hydrogen atoms that are not trapped in vacancy ($D_{non\text{-}trap}$),

$$D_{eff} = D_{trap} \times f_{trap} + D_{non-trap} \times f_{non-trap}$$

and the effect of H/V ratio on the diffusivity of hydrogen is discussed by exploring the overall fraction of the trapped hydrogen atoms (f_{trap}) and the non-trapped hydrogen atoms ($f_{non\text{-}trap}$). In comparison between hydrogen diffusivities given by the model equation and those determined directly with MD simulation, it is revealed that the effective diffusivity of hydrogen is mainly contributed by the hydrogen atoms that are not trapped in vacancy.

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