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Fusion Plasma Modelling Using Atomic and Molecular Data

Summary Report of a Joint ICTP-IAEA Workshop

The *Abdus Salam* International Centre for Theoretical Physics

Trieste, Italy

23–27 January 2012

Prepared by

B. J. Braams

March 2012

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Abstract

The Joint ICTP-IAEA Workshop on Fusion Plasma Modelling using Atomic and Molecular Data was held from 23-27 January 2012 at the *Abdus Salam* International Centre for Theoretical Physics in Trieste, Italy. Ten lecturers presented tutorials and reviews on topics in fusion plasma modelling and atomic, molecular and plasma-material interaction processes. There were 20 participants, generally early-career researchers in the area of A+M+PMI processes and also plasma modellers. The participants presented their work in short talks and a poster session. The proceedings of the workshop are summarized here.

March 2012

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1. Overview

The "ICTP-IAEA Joint Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data" was held the week 23 - 27 January 2012 at the International Centre for Theoretical Physics (ICTP) in Miramare, Trieste, Italy. It followed three earlier related ICTP-IAEA workshops involving plasma modelling and atomic, molecular and plasma-material interaction (A+M+PMI) data:

2009, 20-30 Apr: Joint ICTP-IAEA Workshop on Atomic and Molecular Data for Fusion.
2006, 28 Aug – 08 Sep: Atomic and Molecular Data for Fusion Energy Research.
2003, 08-12 Sep: Workshop on Atomic and Molecular Data for Fusion Energy Research.

The workshop had 10 invited lecturers, 21 other participants, plus the director and the local organizer. The following countries and international organizations were represented (in brackets the total number if more than one): Algeria, Burundi, Cameroon, China (2), Finland, France (2), Germany (6), India (6), Italy (2), Japan, Kazakhstan, Pakistan, Tunisia (3), USA (2); IAEA (2), ICTP.

The aim of the workshop was to bring together plasma modellers that use A+M+PMI data in their work with researchers in the field of atomic, molecular or plasma-material interaction physics that produce relevant data. The workshop was addressed to early-career researchers, generally beyond the level of a Ph.D., that wanted to broaden their outlook with respect to plasma modelling and relevant A+M+PMI processes.

In principle four broad topics are in the domain of the workshop: plasma modelling, atomic processes and spectroscopy, molecular processes, and plasma-material interaction. Within the one-week slot it was not possible to do justice to all four topics and molecular processes received less coverage. Lecturers D. Reiter, K. Ohya and B. Ziaja-Motyka presented plasma modelling, Yu. Ralchenko and H.-K. Chung presented computational procedures for atomic processes and spectroscopy, Yaming Zou/R. Hutton and J. Clementson described EBIT atomic data experiments, M. Telmini spoke on electron-molecule collisions and K. Nordlund, A. Allouche and P. Giannozzi presented plasma-material interaction processes.

The lectures were held in the Euler lecture room in the Leonard da Vinci Building (main building of ICTP); the registration, the poster session and the reception also took place in the Leonardo Building. A computer lab was available for the workshop, but it was not used for the lectures. Some computer code demonstrations were carried out in the Euler lecture room. Most participants stayed in the Adriatico building at ICTP; some stayed in Trieste. The facilities were excellent and the organization was very smooth thanks to the services of the experienced ICTP staff.

Section 2 of this report provides a summary of the lectures and of the short talks and posters. Section 3 provides conclusions and recommendations for a future similar workshop. Appendix 1 contains a list of lecturers and participants. Appendix 2 contains the workshop agenda. Appendix 3 provides the titles of the short talks and posters. Additional workshop materials (including lectures, short talks and posters) are available on the Web; please see these ICTP and IAEA pages:

http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a11151
http://www-amdis.iaea.org/Workshops/

2. Workshop Proceedings

2.1 Introduction

The workshop lasted five days, Mon-Fri. Nine lecturers each had a short lecture (45m) to introduce their field on Monday or Tuesday morning. Tuesday afternoon featured brief (5m) presentations by participants to introduce their work and this was followed by a poster session. The posters remained up through the remainder of the week. A reception was held on Tuesday evening. Therefore, by the end of Tuesday all lecturers and participants had been introduced to the community. Further lectures of up to 90m duration were held Wed-Fri. Section 2.2 provides summaries of all lectures and Section 2.3 provides summaries of the posters. The complete schedule of lectures is provided in Appendix 2 and the titles of the short talks and posters are provided in Appendix 3.

2.2 Lectures

Joe Niemela: Introduction to the ICTP

Dr Joe Niemela (The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy) reviewed briefly the history and function of the ICTP. The ICTP operates under a tripartite agreement between UNESCO, IAEA and the Government of Italy, with most of the funding coming from Italy. The Centre offers Diploma, Masters and Ph.D. programs, post-doctoral appointments, associateships and various fellowships and it offers an extensive yearly programme of schools, workshops and conferences. In addition the centre has a superb library and provides subscription arrangements and electronic access to qualified partner sites. The centre has about 30 permanent scientific staff, 100 long-term scientific visitors per year, 400 short-term visitors and some 6000 participants annually in the meetings programme. Through its funding policies the centre caters especially to visitors from developing countries, but participants in ICTP events come from all over the world.

Detlev Reiter: Edge Plasma Modelling

Dr Detlev Reiter (Institute for Energy and Climate Research, Forschungszentrum Jülich GmbH, Jülich, Germany) presented three lectures on edge plasma modelling with use of fluid and kinetic (Monte Carlo) codes and on the uses of atomic, molecular and plasma-material interaction data in this modelling. After an introduction into magnetic confinement fusion energy research Dr Reiter's lectures focussed on the challenge of particle and power control in ITER and the associated modelling. The ITER edge and divertor is required to exhaust one fifth of the heating and fusion power, i.e. about 100 MW (the rest, 400 MW, is carried by the neutrons) and to exhaust helium ash. Parts of the ITER divertor need to withstand steady power densities of 10 MW/m^2. As a result, the ITER lifetime, performance and availability will not only be influenced, it will be controlled by the physics of the plasma edge region. Edge plasma modelling is a highly interdisciplinary field drawing upon plasma physics, computational fluid dynamics, rarefied gas dynamics, radiation transport physics, and requiring data on atomic and molecular collision processes, plasma-wall interaction processes and opacity. The modelling is multi-scale in space and time and requires macroscopic (generally fluid) and microscopic (generally kinetic) codes.

The underlying equation of the kinetic codes is the celebrated Boltzmann equation and the central tool is the EIRENE Boltzmann solver code. EIRENE is primarily applied to the simulation of neutral gas transport in near-wall plasma, but also radiation transport and transport of charged particles can be handled. The code can be operated as a linear solver or in non-linear mode (including neutral-neutral or photon-neutral collisions). The goal of edge modelling with use of EIRENE and associated fluid codes is to include all of the edge physics that must be operative (opacity, atomic and molecular physics, surface processes, plasma transport), even while our capability to confirm these directly remains limited. Present code effort is directed at low temperature plasma chemistry, improved and consistent wall models, drifts and electrical currents in the edge, a change from 2D to 3D geometry, coupling to first principle edge turbulence codes and integration with core plasma physics codes.

The influence of plasma modelling is seen in the evolution of the design of the ITER divertor: the choice of outside separatrix strike points, a divertor dome to prevent neutrals from penetrating to the core plasma and an optimized pump geometry. The design calls for almost detached plasma operation in which the plasma transitions to a neutral gas in front of the divertor target; as a result the energy deposition on the divertor target is spread radially even if the width of the separatrix plasma channel through which power is conducted into the divertor is only a few mm or as little as 1 mm. Controlling semi-detached plasma operation remains a big challenge, computationally as well as in ITER operation as it is foreseen. The upstream plasma must prevent excessive neutral gas flux into the core plasma also during non-stationary events such as edge-localized modes, as a sudden influx of neutrals into the core could lead to a thermal collapse or even a disruption. Neutral-neutral collisions and Lyman-alpha (and other) photon transport are critical ingredients in the physics of detached plasma.

Dr Reiter concluded his lectures with a review of the atomic, molecular and plasma-material interaction databases associated with EIRENE and collected at http://www.eirene.de. Atomic and molecular data include the HydHel collection for hydrogen and helium, H2vibr for vibrationally excited hydrogen molecules, a set of Jülich reports for hydrocarbon data and Amjuel for other A+M data. The surface data are based upon calculations using the TRIM family of codes. (Please see www.eirene.de for full citations.) The surface data are provided in a format that can be directly used for sampling the probability distribution function in a Monte Carlo calculation.

The databases are supported by an online code HydKin that is intended to expose the data, determine critical reaction paths and explore sensitivities to data errors. HydKin takes as input a number of species and a set of reactions together with densities and temperatures of the background species and initial conditions or source strengths for the selected species. The code then constructs the master rate equation and the evolution of densities of the selected species; in addition it identifies the most important individual reactions and a sensitivity matrix. An example was shown and discussed in some detail where HydKin is used for hydrocarbon atoms and molecules in plasma. At high temperature the critical reactions are all electron impact ionization reactions whereas at low temperature the key reaction channels involve charge exchange with protons followed by dissociative recombination and an increased sensitivity to particle transport details. The HydKin calculation, based on straightforward linear algebra, is also used as a check on the full Monte Carlo code. Finally HydKin is used in order to identify suitable variables for reduced models of the collisional radiative kind.

Kaoru Ohya: Impurity Transport Modelling and Plasma-wall Interaction

Dr Kaoru Ohya (Material and Device Science, Faculty of Engineering, University of Tokushima, Japan) presented two lectures on the subject of modelling erosion and redeposition on plasma-facing walls. The critical issues related to plasma-wall interaction are material erosion, which limits the lifetime of the wall and which is especially severe for light element wall material, impurity production, which causes radiation losses from the plasma and which is especially severe for heavy element wall material, and tritium retention, which constitutes a safety hazard besides removing fuel from the plasma and which is most severe for carbon-based wall material. Processes that must be taken into account include projectile reflection and physical sputtering, chemical sputtering and hydrocarbon emission, impurity deposition and material mixing, thermal diffusion of impurities in materials and transport and redeposition of eroded impurities in the plasma. Modelling of plasma-material interaction is made much more complex due to effects of material migration causing formation of mixed materials and alloys (W-Be, W-Be-C) and changes in surface structure. Impurity transport codes need to treat self-consistently physical and chemical erosion of the surface, transport of released impurities above the surface and through the plasma, redeposition of returning impurities, re-erosion of redeposited impurities and material mixing and alloy formation below the surface.

For the purpose of plasma modelling the plasma-material interaction is generally represented through databases and for erosion most of the data are based upon calculations using the binary collision approximation (BCA) and the TRIM code family due to W. Eckstein. The BCA approach [J. Biersack and H. G. Haggmark, Nucl. Instr. Methods **174**, 257 (1980)] follows only the fast particles in a

collision cascade. These fast particles may undergo deterministic slowing-down in the material and they may collide with atoms in the material in the manner of a local Poisson process. The collisions involve a scattering angle; hard collisions may produce secondary fast particles that are followed in the BCA code whereas for soft collisions only the original particle is followed. When the velocity of a followed particle falls below a threshold then the trajectory is terminated. A trajectory can also terminate because the particle leaves the surface (reflection). Collisions with surface atoms can cause sputtering and so the BCA method is used to calculate trapping, reflection and sputtering.

Chemical sputtering and hydrocarbon emission are low-energy processes that are fundamentally not well described by BCA and for which full molecular dynamics (MD) calculations must be used. The chemical sputtering yield strongly depends on surface temperature and on energy and flux density of bombarding ions. For the purpose of plasma modelling often a description due to J. Roth [JNM266-**269**, 51 (1999)] is used.

Impurity deposition and material mixing may be modelled using a time-dependent version of the BCA (TRIM) approach. For this purpose the material is divided into layers and the composition of each layer is evolved as part of the BCA calculation; the layer width may be changed as well. An example of the use of dynamic BCA is seen in the evolution of carbon deposited on a tungsten surface. Experiments show a sharp change between a region of net erosion and one of net deposition and calculations reproduce that boundary.

For calculating thermal diffusion of impurities in materials an alternative to dynamic BCA is to couple a BCA code to a diffusion code; the BCA code then provides the source term in a diffusion model that is based on Fick's law. The diffusion model may treat impurities as well as defects and vacancies in the material and their interactions [K.L.Wilson, M.I.Baskes, J. Nucl.Mater. **76-77**, 291 (1978)].

Finally the transport of eroded impurities through the plasma and their redeposition on other surfaces involves plasma collision theory (Lorenz force, friction and thermal forces on impurities due to interaction with background plasma), cross-field transport, plasma sheath physics (the electrostatic acceleration through the sheath greatly changes impact properties) and plasma chemistry. For hydrocarbon impurity transport a database containing over 700 reactions is employed. Line emission measurements are available for CH and these measurements together with data on net erosion and redeposition provide critical tests for the integrated modelling of impurity production, transport and redeposition in edge plasma.

In Dr Ohya's second lecture several topics were covered in more detail. A detailed view was provided of integrated modelling of plasma material interaction and impurity transport with use of the EDDY dynamic plasma wall interaction code [K. Ohya and A. Kirschner, Phys. Scr. **T138**, 014010 (2009)]. Comparisons were shown with $^{13}CH_4$ injection experiments done on TEXTOR. Comparisons were shown between calculations done using EDDY and using a particle-in-cell code for hydrocarbon deposition. Molecular dynamics simulations were described for the computation of reflection and sticking coefficients of hydrogen on tungsten, graphite and on W-C mixed material. Some methodological issues with the MD simulations were discussed including the treatment of boundary conditions and the need for a numerical temperature control. Calculations were described of the long-distance transport of beryllium and carbon through plasma; in these calculations essentially all earlier mentioned ingredients of plasma-material interaction and plasma physics are represented. As a final topic calculations of tritium penetration and retention in tungsten were described.

Kai Nordlund: Molecular Dynamics Modelling for Plasma-wall Interaction

Dr Kai Nordlund (Department of Physics and Helsinki Institute of Physics, University of Helsinki, Finland) presented two lectures on atomistic simulations of materials in interaction with plasma using a range of approaches: the binary collision approximation (BCA), molecular dynamics (MD), kinetic Monte Carlo (KMC) and other rate-equation methods and DFT-based quantum calculations.

The physical effects of plasma-material interaction span a wide range of space and time scales, from point processes such as sputtering and the creation of defects to microscale processes such as diffusion of impurities and defects and the formation of clusters, to macroscale processes such as blistering, swelling, crack formation and changes of material properties. The present lectures are concerned with methods for simulations on the smallest scales. An example of a collision cascade due to a fast heavy particle penetrating a thin graphite layer was used to illustrate the nanoscale physics and all the complexity that can be associated with the impact of just a single ion in plasma-material interaction of interest to fusion. The possible effects include formation of a crater, production of sputtered atoms and adsorbed atoms, production of vacancies, point defects and extended defects, amorphization of material and of course ion implantation. For prolonged irradiation many more things can happen, for instance surface roughening and ripple formation, nanocluster, bubble, void or blister formation inside the solid, compositional changes and alloy formation and formation of porous layers known as "fuzz". All these effects are highly relevant for fusion.

The present lectures are concerned with modelling on the atomic level. At this level one needs to handle binary collisions between nuclei at energies up to keV and even MeV as well as energy loss to electronic excitations; this can be done using BCA or using molecular dynamics. The material is locally in transition to high-pressure and high-temperature thermodynamics (solid density, bulk particle energies around 1 eV) and it undergoes phase changes, segregation, sputtering, defect production and other effects. These issues cannot be treated by BCA, but they can still be described by molecular dynamics. Finally the atomistic calculations are used to derive coefficients for kinetic Monte Carlo or rate theory in order to describe long-term processes such as relaxation of defects. The remainder of Dr Nordlund's lectures was given to a systematic exposition of these fundamental computational tools: Binary collision approximation (BCA), molecular dynamics (MD) and kinetic Monte Carlo (KMC) or rate equations.

BCA was developed by Mark Robinson around 1955 and was the original way to treat ion irradiation effects on a computer. (The effect of Channelling was predicted by BCA in these early studies before it was experimentally found.) In BCA the collisions of an incoming ion are treated as a sequence of independent collisions while between collisions the fast particle moves in a straight line or subject to deterministic slowing down (possibly also including effect of small-angle scattering). Collisions can generate new fast particles and particles are removed from the calculation once their energy falls below a threshold. There are variants of implementation: "Plain" BCA that considers only single collision at a time; multiple-collision BCA in which an ion can collide with many lattice atoms at the same time; and full-cascade BCA in which also all recoils are followed. The target material can be static or dynamic; in the latter case the sample composition changes with implantation of incoming ions, ion beam mixing and sputtering. BCA is usually run with amorphous targets ("Monte Carlo" BCA) but with some effort it can also be implemented for crystals. BCA is many, many orders of magnitude more efficient than MD and is very suitable for wide scans of impact and target conditions if one is aware of the limitations. The method is well-suited for fast particle effects and really breaks down at low energies (vicinity of 1 eV) where chemistry becomes important.

MD is solving the Newton's (or Lagrange or Hamilton) equations of motion to find the motion of a group of atoms. It was originally developed by Alder and Wainwright in 1957 to simulate atom vibrations in molecules and this explains the unfortunate name: in fact, MD calculations normally do not involve molecules explicitly and atomic or nuclear dynamics would be a better name. MD studies of radiation effects in solids go back to Gibbons in the 1960s [Phys. Rev. **120**, 1229 (1960)].

In the lecture various timestepping methods were noted as well as timestep selection. Possible boundary conditions include open boundaries, reflecting boundaries, absorbing boundaries or some mixture and the choice is guided by a combination of physical and numerical considerations. Temperature control (thermostatting) and pressure control are critical ingredients of an MD simulation and many algorithms exist, for example the Andersen, Nosé-Hoover, and Berendsen thermostats. Dr Nordlund finds that Berendsen is often to be recommended. The lectures continued with some fine points of MD simulations including adaptive time stepping to handle fast particles in an efficient

manner and the use of dissipative boundary conditions to handle the transition to thermodynamics for high-energy particle impacts.

KMC and rate theory (numerical solution of differential equations) are available for simulations on timescales that are not accessible to molecular dynamics, for example for the relaxation phase after a collision. The starting point for a KMC simulation is an enumeration of all possible transitions used to describe the system and their rates. Each step of a KMC simulation then involves the selection of a single transition according to its probability, application of the transition to the state of the system, and increment of a time variable done in such a way that the algorithm is exact for Poisson processes (processes occurring independent of each other at constant rates). A typical use is atom diffusion for which the transitions are simply atom jumps. The rates need to come from outside the KMC algorithm, for example from experiment, BCA or MD calculations or density functional theory calculations. In the lecture the example of Object KMC for defect motions in solids was used as illustration.

Dr Nordlund described in some detail the construction of interatomic potentials for MD simulations. Ultimately the accuracy of MD is limited by the accuracy of these potentials, so this is a critical ingredient. Relevant concepts include that of a "bond-order" potential and an "embedded atom method" (EAM) potential. The Helsinki group follows a systematic fitting approach introduced by Prof Karsten Albe (TU Darmstadt); see the presentation materials for further pointers. It was carried out at Helsinki largely by Dr C. Björkas for a W-C-Be mixture.

The lectures concluded with a presentation of results of MD simulations of Be, Be-C and W-C mixed divertor materials carried out by the Helsinki group as an example of the possibilities of MD for fusion applications.

Alain Allouche: Density-functional Theory Modelling of Fusion Materials Exposed to Plasma

Dr Alain Allouche (Physique des Interactions Ioniques et Moléculaires, Université de Provence, Marseille, France) provided an introduction to the use of quantum methods for study of plasma-facing materials. Quantum methods must be used when chemical bonds and bond-breaking are involved; so for example for the study of hydrogen trapping, migration and release, defect formation and defect interactions, structure of materials and alloys. Quantum methods are also essential for calculation of density of states (DOS) and solid state spectroscopy.

The most widely used tool for quantum calculations of condensed matter is density functional theory (DFT). The underlying principle for DFT is that the ground state energy of a system of electrons can be expressed as a functional of the electron density (or spin-density), although the functional is not known. In practice DFT relies on approximate functionals inspired by model systems such as a system of non-interacting electrons; this leads to the Kohn-Sham equations, in which there still occurs a functional (the exchange functional) that is not known and for which approximations must be found. A specification of a DFT method therefore involves specification of the basis functions and of the exchange functional.

Typical DFT calculations concern reaction energies and reaction barriers and these calculations involve optimization of a configuration to find local minima and saddle points on the potential energy surface (PES). Examples were discussed of hydrogen bonding in graphite and of the formation of Be-W alloy. These calculations explain the experimental observation that W bonds easily to a Be surface to form an alloy, but Be does not form an alloy in reaction with a W surface. Another example is oxidation of beryllium, which involves dissociation of O_2 as an activated process on the surface. Calculations show the formation of a Be-O oxide layer that tends to dissociate from the beryllium crystal. The final example in Dr Allouche's lecture concerned the energetics of hydrogen and vacancy transport in beryllium and of the interaction between H and vacancies. Tritium trapping in wall material is a serious concern for ITER and for a fusion reactor, and these calculations of the energetics of H and of vacancies in beryllium are critical to the understanding of tritium retention and release.

Paolo Giannozzi: Quantum Simulations of Materials Using *Quantum ESPRESSO*

Dr Paolo Giannozzi (Università di Udine and CNR-IOM Democritos, Trieste, Italy) provided a demonstration of the use of the Quantum ESPRESSO code for some calculations of fusion interest. The basic theoretical tools of materials simulation are DFT and the Kohn-Sham model, use of Pseudopotentials to represent core electrons, and use of Car-Parinello and other iterative techniques for nuclear motion. These tools (sometimes called the Standard Model of materials simulation) were briefly reviewed in preparation for the presentation of the code.

Quantum ESPRESSO ("Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization") is an integrated suite of software for atomistic calculations using density functional theory, a plane-wave basis set and pseudopotentials. The project employs an open source model and seeks innovation in methods and algorithms as well as efficiency on modern computer architectures. The package can be used for structural (static) calculations and energy optimization, dynamical modelling either on the Born-Oppenheimer potential energy surface or using Car-Parrinello dynamics, chemical reactivity and transition path sampling, calculation of linear and some nonlinear response functions, and computational spectroscopy; plus some advanced applications beyond DFT.

The talk then showed actual inputs and results of some model Quantum ESPRESSO calculations inspired by problems of plasma-material interaction. The examples were:

- First-principles study of neutral silicon interstitials in 3C- and 4H-SiC
- Energetics and metastability of the silicon vacancy in cubic SiC
- Evidence for a kinetic bias towards antisite formation in SiC nano-decomposition
- Stoichiometric Defects in Silicon Carbide
- Activation entropies for diffusion in cubic silicon carbide from first principles
- Ab initio investigation of radiation defects in tungsten: Structure of self-interstitials and specificity of di-vacancies compared to other bcc transition metals
- Quantum modelling (DFT) and experimental investigation of beryllium-tungsten alloy formation

For the purpose of the demonstrations only very small basis sets and lattice sizes were employed; nevertheless the results were in each case quite reasonable. The examples demonstrated the ease with which the problem specifications can be prepared for Quantum ESPRESSO.

Yuri Ralchenko: Atomic Collisions and Spectroscopy

Dr Yuri Ralchenko (Atomic Spectroscopy Group, National Institute of Standards and Technology, USA) presented three lectures on atomic spectroscopy in plasma, emphasizing those aspects that are important for plasma diagnostics. The first lecture provided an overview of concepts of atomic structure and radiative processes. The second lecture provided a more detailed exposition of the important elementary processes and the third lecture was devoted to thermodynamic considerations relevant for spectroscopy.

In the first lecture basic concepts of atomic structure and spectroscopy were introduced. The major sources of photons are free-free transitions, $A^{z+} + e \rightarrow A^{z+} + e + h\nu$, free-bound transitions (radiative recombination), $A^{z+} + e \rightarrow A^{(z-1)+} + h\nu$, and bound-bound transitions, $A_j^{z+} \rightarrow A_i^{z+} + h\nu$. All are important for plasma diagnostics and for the energy balance in plasma. For a transition from state *j* to state *i* belonging to the same ion the power density is given by the expression $I_{ij} = N_j \cdot A_{ij} \cdot E_{ij}$ in which N_j is the upper state density, A_{ij} is the Einstein coefficient or transition probability (per unit time) and E_{ij} is the energy of the transition (the photon energy). The Einstein coefficient and the transition energy are to first approximation purely atomic parameters while the level population density is determined by the interaction with the plasma environment.

The simplest system for atomic structure is the hydrogen atom or hydrogen-like ion. Radiative processes involve excited states and in many cases (in particular for Rydberg states) it is appropriate to treat an ion of charge Z as a core of charge Z+1 and one hydrogen-like electron. This justifies the concept of "spectroscopic charge" z=Z+1 and the spectroscopists' notation, e.g. Ar III for Ar^{2+}.

For the hydrogen or hydrogen-like ions the level energies are characterized by only the principal quantum number *n*. Beyond the simplest model electron-electron interaction, spin-orbit interaction and other terms create a more complicated level structure. In the lecture it was explained how different types of interaction result in different couplings. For instance, the so-called LS coupling reflects strong electron-electron interation terms in the Hamiltonian whereas the jj-coupling points out to importance of spin-orbit interaction. These concepts give rise to different, alternative schemes for labelling electronic states when these (and other) terms are present in the Hamiltonian. In addition it must be kept in mind that the solution of a many-electron Schrödinger equation is not, in general, a pure state; there is configuration interaction and state mixing.

The quantum electrodynamics gives rise to a classification of radiative transitions in terms of electric or magnetic multipoles and it leads to the concepts of selection rules and of allowed and forbidden transitions. These concepts were introduced in Dr Ralchenko's first lecture and it was explained how "forbidden" transitions can in fact be quite strong.

In his second lecture Dr Ralchenko described in more detail the elementary radiative and collisional processes that are relevant to atomic spectroscopy in plasma. These processes include radiative decay, dielectronic capture and dielectronic recombination, autoionization, radiative recombination, collisional excitation and ionization, excitation-autoionization, three-body recombination, and some heavy particle collision processes. Some popular codes and databases were briefly discussed too, but the focus was on theory.

Radiative decay was discussed with special empahsis on forbidden transitions which are often used in plasma diagnostics. The presentation was illustrated with the examples of the aurora borealis and of emissions from highly charged tungsten in fusion plasma. The green light of the aurora borealis is due to an E2 forbidden transition in atomic oxygen and in the tungsten example most strong lines are associated with M1 transitions. These phenomena were explained with reference to the relevant level schemes and lifetimes.

Selection rules for radiative decay are again important in the study of autoionizing transitions and this has a key role in the process of dielectronic recombination (DR). Dielectronic recombination is a two-step process: capture of a free electron by (resonant) excitation, followed by radiative decay. For the second stage autoionization is a competing process; it is inverse to the original dielectronic capture.

Collisional excitation occurs primarily due to electron collisions and the processes can be classified as optically (dipole)-allowed, optically-forbidden and spin-forbidden. Typical cross-sections were shown together with their scaling as a function of electron energy. The scaling of the cross section with principal quantum number *n* was discussed and the significance of the (formally indistinguishable) direct and exchange channels and of resonances.

Dr Ralchenko's third lecture was concerned with equilibrium distributions of atomic states in plasma, with conditions for the establishment of full or partial equilibrium and with spectroscopic properties of atomic systems in (partial) equilibrium. For the purpose of atomic physics there are four primary populations to consider and each of these may be in thermodynamic equilibrium or not. For photons the equilibrium distribution is the Planck distribution. For electrons it is the Maxwell distribution. For the level population within a given atom or ion it is the Boltzmann distribution and for the charge state balance it is the Saha distribution. In pure thermodynamic equilibrium all these distributions are established and all at the same temperature. Detailed balance applies too; the rate of each process is balanced by that of its inverse process.

In the laboratory one never has a full thermodynamic equilibrium, because the photons are untrapped. The situation in which photons are untrapped and all else is in equilibrium is described by the name local thermodynamic equilibrium (LTE), which therefore means a Maxwell distribution for electrons, Boltzmann distribution for excited states and Saha distribution for charge states, all at the same temperature. For calculation of LTE populations the only atomic data that are needed are energies and statistical weights. Transition rates are not needed to calculate the equilibrium, but they are needed to calculate radiative energy loss. Various criteria (Griem's and Saha's) for the validity of LTE were explained in the lecture.

At low density another simplification applies when radiative lifetimes (which are independent of density) are short relative to collisional lifetimes. This limit is called the coronal regime and the distribution is called coronal equilibrium. In the coronal limit the population density of excited states is small; multistep excitation or ionization processes are not relevant (except for a possible presence of metastable states) and the population density of excited states is only required to calculate radiative loss rates. Note that in coronal equilibrium radiative decay can still be a multistep process (a cascade).

In the coronal regime the principal processes that change an ion charge are all directly proportional to electron density and therefore the ratio of charge state densities N^{Z+1}/N^Z is independent of density. In the Saha equilibrium, at higher density, 3-body recombination dominates and $N^{Z+1}/N^Z \sim 1/N_e$.

The regime intermediate between coronal equilibrium and LTE is the domain of collisional radiative (CR) modelling that is discussed in these lectures by H.-K. Chung. Some concepts of equilibrium continue to apply and this is reflected in the concept of partial LTE (PLTE). As a function of principal quantum number the rate of radiative decay decreases as $1/n^{4.5}$ while the rate of collisional excitation or deexcitation increases as n^4. As a consequence one may assume that LTE applies for Rydberg states at sufficiently high n even as the lower excitation levels are described using the collisional radiative model or the coronal model.

Dr Ralchenko concluded his lectures with a presentation of the effect of density from the coronal to the LTE regime on the emission intensity of spectral lines and the use of measured line ratios as diagnostic of density and/or temperature in fusion experiments. Emissions from He-like Ar and from H-like Ne were used as an example.

Hyun-Kyung Chung: Collisional-radiative Modelling

Dr Hyun-Kyung Chung (International Atomic Energy Agency, Vienna, Austria) gave two lectures on modelling of atomic processes in plasma and theoretical plasma spectroscopy. The range of plasma conditions studied by spectroscopy is enormous, temperature varying from 10^{-6} K to 100 keV (10^9 K) and density varying from $10^5/\text{cm}^3$ – $10^{23}/\text{cm}^3$ as one considers the interstellar medium, solar corona, various terrestrial plasmas, magnetic fusion, inertial fusion and stellar interiors. Theoretical plasma spectroscopy aims to understand radiation from these sources and it requires a wide range of tools and theories both from quantum physics (atomic physics, collision physics, line shape theory) and classical physics (radiation transport, hydrodynamics, plasma kinetic theory).

The basic atomic data start from the atomic level structure and involve bound-bound and bound-free transitions:

- $A_1 \rightarrow A_2 + h\upsilon_2$ (spontaneous emission)
- $A_1 + h\upsilon_1 \leftrightarrow A_2 + h\upsilon_1 + h\upsilon_2$ (photo-absorption or emission)
- $A_1 + e_1 \leftrightarrow A_2 + e_2$ (collisional excitation or deexcitation)
- $B_1 + e \rightarrow A_2 + h\upsilon_3$ (radiative recombination)
- $B_1 + e \leftrightarrow A_2 + h\upsilon_3$ (photoionization and stimulated recombination)
- $B_1 + e_1 \leftrightarrow A_2 + e_2$ (collisional ionization and recombination)
- $B_1 + e_1 \leftrightarrow A_3 \leftrightarrow A_2 + h\upsilon_3$ (dielectronic recombination: autoionization + electron capture)

These transitions are coupled in a population kinetics model that describes in principle the population balance in the complete level structure of any charge state of any ion. The key is to figure out how to manage the infinite set of levels and transitions of atoms and ions into a model with a tractable set of levels and transitions that represents physical reality. The local population kinetics model is in turn coupled to a radiation transport model that requires data on opacity and emissivity, which in their turn require population densities and radiative transition probabilities. In addition the radiation transport requires line shape models: a theoretically rich field incorporating quantum mechanics and statistical mechanics. Line shapes (natural broadening, Doppler broadening, Stark broadening, opacity broadening and resonance broadening) also provide diagnostics for a vast range of plasma conditions. Finally the atomic physics and radiation transport may all be incorporated into hydrodynamics simulations or Particle-In-Cell (PIC) simulations.

The rate equations that determine the level population distribution may be simplified somewhat in two opposite limiting cases: that of low-density "coronal" plasma and that of high-density plasma in local thermodynamic equilibrium (LTE). In the coronal limit excited state population densities are so low that it may be assumed that they are populated only directly from the ground state by collisional excitation and depopulated by spontaneous emission; the process of excitation from one excited state to a higher excited state can be ignored. The excited population density is then proportional to electron density n_e and the charge state distribution is independent of n_e. In the LTE limit population and depopulation processes are dominated by collisions including 3-body recombination; hence the high-lying states are important for charge state balance and the population distribution is an explicit function of local plasma conditions governed by Boltzmann statistics and Saha equations.

For plasma conditions between the coronal and the LTE limits the level population distribution must be determined by solving rate equations that couple population densities in ground and excited states and that include both collisional and radiative processes. This is the field of non-LTE (NLTE) kinetics and collisional-radiative modelling. Stepwise ionization through excited states and 3-body recombination must be included in the model together with radiation transport, fast particle collisions and density effects. For optically thick lines self-absorption reduces the radiative processes and must be included too.

In the remainder of the introductory lecture Dr Chung discussed some specific processes that are included in NLTE calculations, notably dielectronic recombination and stepwise excitation.

Dielectronic recombination (DR) is the process in which an electron and ion combine and the recombination energy is at first taken up by excitation of another bound electron. The resulting state is autoionizing, but it can also decay by radiation. In the intermediate density regime DR is usually the dominant recombination process (to be compared with radiative recombination at low density and 3-body recombination at high density). Results of calculations of DR depend very much on the number of channels included in the calculation as was shown through several examples in the lecture.

Stepwise excitation is important in the NLTE regime and it causes the excited level population densities and radiative loss rates to depend in a nonlinear way on n_e as was illustrated in the lecture by calculations of radiative cooling of Kr in plasma. In higher density plasma calculations of the 3-body recombination processes require a careful treatment of highly excited states due to the continuum lowering or ionization potential depression by interaction with neighbouring atoms in the plasma.

In her second lecture Dr Chung showed examples of non-LTE modelling for plasmas generated in fusion and other applications. A non-LTE kinetics code FLYCHK [H. Chung et al., High Energy Density Physics **1**, 3 (2005)] was applied to predict ionization distributions and spectral characteristics of finite density plasmas. Results were presented for charge balances and spectra of high-Z plasmas generated by a long-pulse laser, charge balances of photo-ionized plasmas, K-alpha emission due to energetic electrons generated by short-pulse lasers, time-dependent spectra of plasmas generated by x-ray free electron lasers and radiative cooling rates of plasmas over a wide range of plasma conditions.

The examples were published in a review article [H. Chung and R. Lee, High Energy Density Physics, **5**, 1 (2009)].

The proceedings of a sequence of code comparison workshops on non-LTE modelling, for example [C.J. Fontes et al., High Energy Density Physics **5**, 15 (2009)], are a rich source of further information and examples. The most recent workshop in the series was held in Vienna in December 2011 [http://nlte.nist.gov/NLTE7/].

Beata Ziaja-Motyka: Modelling of Warm Dense Matter

Dr Beata Ziaja-Motyka (Center for Free-Electron Laser Science, DESY, Hamburg, Germany) presented two lectures on modelling of warm dense matter and the transition from condensed matter to warm dense matter regime. Free-electron lasers such as FLASH at DESY and the European X-ray Free-Electron Laser (XFEL) now under construction can probe matter at atomic length scales and femtosecond (10^{-15} s) resolution. Dr Ziaja's first lecture focussed on physical processes in samples irradiated by VUV, soft- and hard X-rays. The second lecture focussed on modelling with use of Monte Carlo (MC) codes, Boltzmann codes, and integrated electronic structure (tight-binding DFT), molecular dynamics, Monte Carlo and Boltzmann models. This work is done in the CFEL Theory Division where the research interests include the dynamics of excited many-electron systems, the motion of atoms during chemical reactions and X-ray radiation damage in matter.

A sample that is irradiated by an intense FEL pulse evolves in two main phases: a non-equilibrium ionization phase that lasts until thermalization of electrons is reached followed by an expansion phase in which the electron plasma is in local thermodynamic equilibrium that slowly equilibrates with the ion population. Basic processes include photoionizations and collisional ionizations, elastic scattering of electrons on atoms and ions, long-range Coulomb interactions of charges with external and internal fields, heating of electrons by inverse bremsstrahlung, modification of atomic potentials by electron screening and ion environment, dielectronic and 3-body recombination and short range electron-electron interactions. Other processes may contribute as well: multiphoton (multistage) ionization, many-body recombination and ionization by internal electric field. The plasma evolves from a strongly coupled degenerate plasma, which is fundamentally a many-body quantum system, to a classical ideal warm plasma. In some works the degenerate plasma is actually treated in a quantum kinetic approach, but also semi-classical models are used. These must include dense plasma effects such as quasiparticle self-energies, lowering of continuum level and of ionization thresholds and changes in photo-, collisional and recombination thresholds due to charge screening.

Several physical processes were described in some more detail in the introductory lecture; in particular inverse bremsstrahlung and the Auger effect in photoionization.

The second, longer lecture was devoted to methods for modelling the warm dense matter. Well-established methods are based on classical or semi-classical models using a particle approach (Monte Carlo, deterministic molecular dynamics, particle-in-cell simulations) or using a continuum transport model (Boltzmann equation in phase space or hydrodynamic models). In the lecture several examples were discussed of the use of particle or Boltzmann methods:

- Monte Carlo modelling of an Auger electron cascade [e.g., B. Ziaja, R. A. London and J. Hajdu, J. Appl. Phys. **97**, 064905 (2005)].
- Monte Carlo code to follow electron dynamics within FLASH irradiated aluminium [N. Medvedev et al., Phys. Rev. Lett. **107**, 165003 (2011)].
- Boltzmann simulations of atomic clusters under FEL irradiation [B. Ziaja et al., Phys. Rev. Lett. **102**, (2009); B. Ziaja et al., New J. Phys. **11**, 103012 (2009)].
- Modelling of soft X-ray Thomson scattering in warm dense hydrogen.
- Modelling of ionization balance in irradiated mixed clusters (Xe/Ar).

The lecture continued with a discussion of integrated quantum-classical modelling, combining Monte Carlo, molecular dynamics, tight-binding DFT and a Boltzmann approach to study structural changes in solids following irradiation (work by N. Medvedev, H. Jeschke and B. Ziaja). In this combined approach the motion of ions and atoms is described by molecular dynamics, electrons within the valence and conduction bands are described by the Boltzmann equation, the band structure and the potential energy surface are obtained by tight binding DFT, high energy free electrons and the creation and relaxation of core holes are modelled using a Monte Carlo approach, and rates for scattering and ionization are calculated from complex dielectric function updated at each time step. In conclusion some challenges and perspectives were discussed for further modelling of warm dense matter produced by FEL irradiation.

Mourad Telmini: Electron-molecule Collisions

Dr Mourad Telmini (Department of Physics, Faculty of Science of Tunis, and National Centre for Nuclear Science and Technology, Tunisia) gave two lectures on computations of electron-molecule collisions. The case of reactions of H_2^+ + e was used as a prototype. Already for this simple case there are several reaction channels to consider:

- $H_2^+(v) + e \rightarrow H_2^+(v) + e$ (elastic collision)
- $H_2^+(v) + e \rightarrow H_2^+(v') + e$ (inelastic collision, v'>v)
- $H_2^+(v) + e \rightarrow H_2^+(v') + e$ (superelastic collision, v'<v)
- $H_2^+(v) + e \rightarrow H + H$ (dissociative recombination)
- $H_2^+(v) + e \rightarrow H^+ + H + e$ (dissociative excitation)
- $H_2^+(v) + e \rightarrow H^+ + H^+ + 2e$ (dissociative ionization)

The processes proceed through an H_2 intermediate state in the continuum and calculations require an ab initio characterization of this excited and doubly-excited molecular hydrogen.

The relevant highly excited states of H_2 can often be pictured as a Rydberg (high-*n*) electron around an H_2^+ core, which is not so different from an atomic system having a single valence electron. Therefore to introduce treatment of highly excited molecular states first the structure of hydrogen and of alkali atoms is reviewed. The Schrödinger equation for the hydrogen atom is exactly solvable and one finds energy levels depending only on the principal quantum number, $E_n = -1/2n^2$ in atomic units. As was found by Rydberg (1899) alkali atoms have a similar level structure. The angular quantum number l enters and in present notation the Rydberg series have the form $E_{nl} = -R/(n-\delta_{nl})^2$ where δ_{nl} is called the quantum defect following R. J. Seaton. The quantities δ_{nl} correspond to phase shifts in the electron wavefunction. Single channel quantum defect theory considers the interaction among a single pair of electrons whereas multichannel quantum defect theory considers the interaction of one (Rydberg) electron with multiple core electrons.

The matching of the electronic wavefunction between the asymptotic region and the core is described by R-matrix theory, first developed by E. P. Wigner to describe resonances in nuclear collisions and developed in variational form by W. Kohn. Applications in atomic physics of the combination of multi-channel quantum defect theory and the variational eigenchannel R-matrix were developed especially by Greene and Aymar; see their review of multichannel Rydberg spectroscopy of complex atoms [M. Aymar, C. H. Greene and E. Luc-Koenig, Rev. Mod. Phys. **68**, 1015 (1996)].

In his second lecture Dr Telmini showed the application and extension of these ideas to Rydberg molecular systems and electron-molecule collisions. Starting point is the Born-Oppenheimer approximation, separating the electronic structure from the nuclear motion, and this was briefly reviewed. The lecture then focussed on the *halfium model*, which combines the variational eigenchannel R-matrix method and a generalized multichannel Quantum Defect Theory (GMQDT) and which uses a "halfium particle" as the one-electron reference system to describe the molecular core. The approach is motivated by the case of H_2^+ + e scattering, for which the core is a true single-electron system, but in a more approximate manner it is also applied to other binary molecules.

The halfium particle has two-center symmetry and the electric field and wavefunction are described in prolate spheroidal coordinates. For the case of H_2^+ the charge is modelled following R. S. Mulliken as a charge of ½ on each of the two nuclear centres, hence the "halfium" name. The wave equation is separable in the prolate spheroidal coordinates and the phase-amplitude formalism can be carried through using Generalized Coulomb functions in a similar way as for an atomic system [M. Telmini and Ch. Jungen, Phys. Rev. A **68** 062704 (2003)]. In the lecture several applications to H_2 and the H_2^+ + e scattering problem are described in more detail, and one may see also the short talks and posters at this workshop by F. Argoubi and H. Oueslati.

Yaming Zou, Roger Hutton and Joel Clementson: Electron Beam Ion Trap Experiments

The original schedule called for an introductory lecture by Dr Yaming Zou on Monday about EBIT experiments followed by three short lectures by the three listed speakers later in the week on specific topics related to EBITs. Dr Zou had prepared her lectures, but had to cancel her participation at the last moment. Her prepared lectures were presented by Dr Hutton.

The introductory lecture by Dr Yaming Zou (Shanghai EBIT Laboratory, Modern Physics Institute, Fudan University, Shanghai, China) described the principles of an Electron Beam Ion Trap (EBIT) and its uses to assist fusion plasma diagnostics. In an EBIT an electron beam is produced at an energy of up to several 100 keV. The space charge of the electron beam traps ions, which are produced by repeated collisions with the beam electrons. EBIT experiments have been around since 1986 (the Livermore Super EBIT). The early ones rely on helium-cooled superconducting magnets, but more recently also compact EBITs employing permanent magnets have been introduced and these are truly table-top experiments. Before the advent of the EBIT ions with charge states higher than 30 could be produced only on very expense high energy accelerators. Now the EBIT can easily produce these ions, in essentially any charge state of any element up to helium-like or hydrogen-like uranium excluding only the lowest charge states. (If the beam energy is below about 100 eV then dispersion due to space charge is too large and the beam cannot be focussed.) The EBIT is an excellent tool for both collision experiments and spectroscopic studies.

The EBIT may be used as a source of highly charged ions (HCI) for collision experiments. The ions are extracted, accelerated, passed through an analysing magnet and then decelerated to the desired energy and passed into a collision chamber. At Fudan the key analysis technique for collisions is the Recoil-ion and electron momentum spectroscopy. Post-collision ions and electrons are detected in coincidence, which allows almost full-information measurements of HCI-ion, HCI-atom, HCI-electron and HCI-photon collisions. Also HCI have been used to create extreme states of matter by "Coulomb explosions" when an HCI (up to hydrogen-like uranium) is brought in contact with a surface.

EBITs provide an excellent tool for spectroscopic studies because although the ions are highly charged they are motionally cold and the lines are sharp (typical width below 1 eV). Detailed studies rely on scans of electron beam energy that allow to pinpoint accurately the onset of any line and thereby identify the relevant level structure and branching ratios. In the lecture an example was presented involving the level structure of Li-like Ar^{15+} and He-like Ar^{16+} and another example involving emission from moderately charged tungsten ions, down to W^{10+}.

In her second lecture Dr Yaming Zou described the use of EBITs for studies of dielectronic recombination (DR). In the DR process a free electron is captured by an ion and the excess energy is initially taken up by exciting a bound electron. This leads to a doubly excited state above the continuum of the recombined ion. The DR process is complete when the doubly excited ion stabilizes via photon emission. DR is a resonant process which only happens when the free electron's kinetic energy matches the energy difference between the doubly excited state and the initial state. DR processes play a key role in determining the charge state balance in hot plasmas and are also the main cause of satellite lines.

Because DR is a resonant process one studies it by scanning the electron beam energy and observing photon emission and, if possible, change in charge balance. The energy scan may be classified as either slow or fast relative to the timescale for changing the ionization balance among the trapped ions. The mathematical analysis of the data starts from the full time-dependent kinetics and simplifies in the slow and fast limits. If a slow scan is done then the ion population is in equilibrium with the beam energy while in a fast scan the population balance is as it has been prepared before the scan. The fast scan technique makes it possible to measure DR for electron collision energies much below the ionization energy; i.e., for collisions with electrons from the low-energy part of the distribution function in a plasma.

As an example of the use of slow scanning to measure DR Dr Zou described a study for highly charged xenon using the Shanhai EBIT [W. D. Chen et al., Phys. Plasmas 14, 103302 (2007); W. D. Chen et al., Phys. Plasmas **15**, 083301 (2008)]. A subsequent study of the same system used the fast scanning technique to explore other DR resonances [K. Yao et al., Phys. Rev. A **81**, 022714 (2010)].

Dr Roger Hutton (Shanghai EBIT Laboratory, Modern Physics Institute, Fudan University, Shanghai, China) discussed uses of atomic spectroscopy for plasma diagnostics and uses of the EBIT for atomic spectroscopy. Lineshapes and relative intensities of radiation from ions in plasma are influenced by electric and magnetic fields and by the plasma environment and this underlies plasma diagnostics based on atomic spectroscopy. Most often metastable levels are involved and usually a line ratio is used. As a historical example the case of the solar corona green line at 5302.86 Å was discussed, which was explained in the 1940s as a $^2P_{1/2} - {}^2P_{3/2}$ ground state forbidden transition in Fe XIV (Fe^{13+}). More recently, in 1978 photons from forbidden M1 transitions in Fe XX were observed in the Princeton tokamak and the authors could determine the ion temperature to be around 45 MK. For some time the tokamak actually became an important light source for spectroscopic studies.

Dr Hutton used examples from Be-like N to explain how line intensity ratios are sensitive to electron density so that the spectroscopy can be used as an electron density diagnostic. For tokamaks the relevant ratio involves transitions from levels of the $2s2p\ ^3P$ term to the $2s^2\ ^1S_0$ ground state. As an example of the possible complexity of these line ratio diagnostics the case of some M3 lines in Ni-like Xe was discussed. The magnetic octupole line is influenced by nuclear spin and the intensity changes by a factor of about 5 as one switches from natural Xe to isotopically pure ^{132}Xe.

Dr Joel Clementson (Lawrence Livermore National Laboratory, USA) described the practice of EBIT spectroscopy using tungsten as the example. Due to its high melting point, low tritium retention, high energy sputtering threshold and low sputtering yield tungsten is favoured as a plasma-facing material. It is the chosen material for the ITER divertor; the AUG tokamak in Garching, Germany, operates with an all-tungsten wall and the JET tokamak in the UK now has a tungsten divertor. Atomic data for tungsten are highly desired and EBIT spectroscopy is perfectly suited for producing these data. By comparison with the tokamak environment the EBIT has a wider energy range (30 eV – 200 keV), much less Doppler broadening (normally below 1 eV), cleaner composition (single impurity only) and the possibility to isolate specific processes by tuning the beam energy. All charge states of tungsten (Z=74) can be produced in an EBIT.

The precision of EBIT spectroscopy is well illustrated by spectra in the EUV range, 30 – 70 Å. Spectra taken on the ORMAK (ORNL) and PLT (Princeton) tokamaks in the 1970s and on Alcator C-Mod (MIT) in 2011 show densely spaced line emission from n = 4 – 4 transitions from tungsten ions of many charge states. A slow energy scan in the EBIT shows individual lines appearing and disappearing as a function of beam energy. With support from atomic structure calculations this makes it possible to assign essentially every line in the observed spectrum.

As was discussed already by Dr Zou EBITs are also used to study emission due to two-body recombination processes: dielectronic recombination (DR) and radiative recombination (RR). DR and RR are important line-formation mechanisms in EBIT plasmas and are important for the ionization balance in fusion plasmas.

The LLNL EBIT group produces reference atomic data for ITER diagnostics based on spectroscopy of tungsten. X-ray transitions n = 2 – 3 in tungsten are the physics basis for the ITER Core Imaging X-ray Spectrometer and ion temperature and plasma-rotation profiles may be obtained from Doppler broadening and shifts of W x-ray lines. Specific levels and transitions of interest for ITER core diagnostics involve tungsten L-shell ions (Ne-like W^{64+} – Li-like W^{71+}). Within these ions there are several groups of strong x-ray transitions that have been measured on the LLNL SuperEBIT:

- $2p_{1/2} – 2p_{3/2}$ M1 and E2 transitions, 1200 – 1500 eV
- $2s_{1/2} – 2p_{3/2}$ E1 transitions, 1600 – 1900 eV
- $2p_{3/2} – 3s_{1/2}$ E1 (and M2) transitions, 8000 – 9000 eV
- $2p_{3/2} – 3d_{5/2}$ E1 transitions, 9000 – 10000 eV

In addition to these fundamental transitions high-order multipole (forbidden) transitions can produce strong lines in tokamak plasma that are important for charge-balance modelling and can be used for electron-density diagnostics. Magnetic dipole (M1), electric quadrupole (E2), and magnetic octupole (M3) transitions in W have been studied at several EBIT laboratories including LLNL and NIST and some spectra were shown in the talk.

2.3 Short Talks and Posters

Fatma Argoubi, LSAMA Department of Physics, Faculty of Science of Tunis, University of Tunis, Tunisia: *Ab-initio computation of excited states of molecular hydrogen: Halfium model*. (Joint work with S. Bezzaouia, H. Oueslati, M. Telmini, Ch. Jungen, I. F. Schneider and O. Motapon.) Rydberg and doubly-excited states of the H_2 molecule are investigated. The molecule is treated in a collisional approach as consisting of an H_2^+ ionic core and an external electron that can be in a Rydberg or a continuum state. The wavefunction of the Rydberg electron is expanded in spheroidal coordinates. A variational R-matrix approach combined with multichannel quantum defect theory is used following [M. Telmini and Ch. Jungen, Phys. Rev. A **68**, 062704 (2003)]. Several Rydberg series converging to the $2p\pi$ state of the H_2^+ ion core are established and their mutual channel interactions characterized; these results were published in [F. Argoubi et al, Phys. Rev. A **83**, 052504 (2011)]. Now these structure calculations are being applied for calculation of cross-sections and rate coefficients for dissociative recombination. First results are shown in the poster.

Gunnar Bandelow, Max-Planck-Institut für Plasmaphysik Teilinstitut Greifswald, Germany: *Simulations of low-temperature plasmas*. (Ph.D. research supervised by Profs R. Schneider and J. Meichsner.) The work is devoted to simulated of a capacitively coupled radio frequency CF_4/H_2-discharge in the laboratory of Prof Meichsner with focus on the plasma chemistry. Relevant species include the CF_x chain and their ions, H_2^+, atoms C, F, H and their ions C^+, F^+ and H^+, also negative ions such as F^- and CF_3^-, and larger molecules and ions in the C_xF_y family. Reactions include dissociation by electron impact, charge transfer, mutual neutralization, three-body recombination. All in all more than 40 species and more than 200 reactions are considered. Much of the effort is devoted to assembling the database of reaction cross-sections and rate coefficients. Comparisons are shown between 0d calculations of chemistry with results of a flow-tube experiment.

Muhammad Abbas Bari, Pakistan Atomic Energy Commission: *Calculation of radiative properties of hot dense plasmas*. The objective of the work is to study opacity of plasma, which requires data for radiative processes, electron collision processes and lineshapes. Codes GRASP2 and FAC were used to calculate energy levels, transition rates, oscillator strengths and lifetimes in Ne-like Au [M. A. Bari et al., J. Phys. B: At. Mol. Opt. Phys. **44**, 225004 (2011)]. More recently the DARC code was used for relativistic calculations of line broadening by electron impact in beryllium-like ions. A three-ion collisional-radiative model was developed to simulate non-LTE emission and absorption spectra.

Zeyneb Bedrane, Laboratoire de Physique Théorique, Dpt. Physique, Université de Tlemcen, Algeria: *How anisotropic electrons influence the density diagnostic of hot plasma?* We have theoretically investigated how a small fraction of energetic beamed electrons influences the diagnostics of the

electron density in hot plasmas, based on the intensity ratio R of the helium-like forbidden line to the intercombination lines. Elaborate calculations of the intensity ratio R have been performed for Ne^{8+} ions over the range of electron densities 10^9–10^{13} cm^{-3} using an electron distribution (model) that includes both Maxwellian isotropic and monoenergetic beam components. By taking into account all important transitions among the 117 magnetic sublevels of the $1s^2$ and 1snl (n = 2–4) configurations, a collisional-radiative model has been applied for determining the populations of the upper-magnetic sublevels of lines. The required collision strengths due to both electron components were computed semi-relativistically in the complementary distorted-wave and Coulomb–Bethe methods. The results are given for temperature of the Maxwellian electron component in the range $2–5 \times 10^6$ K and for kinetic energies of the monoenergetic electron component between 0.95 and 4 keV. The electron density inferred from the intensity ratio R without including the beam effect can be significantly overestimated or underestimated depending upon the emission angle relative to the electron beam direction [Z. Bedrane, M. K. Inal and S. Fritzsche, J. Phys. B: At. Mol. Opt. Phys. **42**, 055701 (2009)].

Bastiaan Braams, Nuclear Data Section, IAEA, Vienna, Austria: *Work of the IAEA A+M Data Unit on atomic, molecular and plasma-surface interaction data for fusion*. The mission of the IAEA atomic and molecular data unit is to provide evaluated and recommended databases of atomic, molecular and plasma-material interaction properties and to some extent materials properties relevant to fusion energy. To this end the unit organize meetings, workshops and coordinated research projects, develops and maintains databases and data exchange standards, coordinates an international Data Centres Network and generally supports data evaluation and data and code exchange activities. The poster provides an overview of the coordinated research projects, data development projects, meetings and workshops organized by (or in collaboration with) the unit and of the bibliographical and numerical databases and the wiki-style knowledge base maintained by the unit.

Kalyan Kumar Chakrabarti, Department of Mathematics, Scottish Church College, Kolkata, India: *Dissociative recombination and excitation in H_2^+, HD^+ and BeH^+*. The MQDT method is used to calculate dissociative recombination and excitation. Two types of dissociative excitation are considered [K. Chakrabarti et al., AIP Conf. Proc. **1387**, 37 (2011)]: in the DE1 process the molecular ion is excited from an initial vibrational state to the continuum and in the DE2 process it is excited from an initial vibrational state to a repulsive excited state of the ion. The work on H_2^+ and HD^+ is completed and that on BeH^+ is underway [K. Chakrabarti and J. Tennyson, EPJ D **66**, 1 (2012)].

Julia Duras, Ernst Moritz Arndt Universität Greifswald, Greifswald, Germany: *Particle simulation of ion thrusters*. (Ph.D. research supervised by Prof R. Schneider.) The presented work shows numerical simulations to study the physics of high-efficiency multistage plasma thrusters (HEMP-Ts) built by the Thales Group. It tries to contribute to an improved understanding of the basic effects needed to optimize such systems. Two major topics are shown, a Particle-in-Cell (PIC) simulation of the channel plasma and the problem of plasma-wall interaction during terrestrial testing. In both topics atomic data has been used to simulate particle-particle interactions and sputter yields. The PIC simulations show a nearly constant plasma potential with a steep drop at the exit zone and an electron distribution that touches the channel walls only in the narrow "cusp regions" of the thruster. Different potential and particle distribution in the Stationary Plasma Thruster (SPT) result in very different erosion characteristics due to energetic ions hitting the walls. In a comparison the SPT shows rather strong erosion whereas HEMP has nearly negligible one. The second topic concerns simulation of the interaction of ions in the plume region with test vessel walls and back-flow of impurities generated by this process; this backflow can produce artifacts in measurements of thrust and of angular distributions of the emitted ions. Calculations of backflow of impurities from the vessel walls are presented using Monte-Carlo and analytical approaches. The approaches agree very well and support the experimental results. Based on these models implementation of tilted baffles in testing devices is proposed, which will be realized soon in industry.

Michel Douglas Epée Epée, Departement of physics, Faculty of science, University of Douala, Douala, Cameroon: *Rotational transitions induced by collisions of H_2^+ ions with low energy electrons.* In this work we use the Multichannel Quantum Defect Theory (MQDT) [I. F. Schneider et al., J. Phys.

B: At. Mol. Opt. Phys. 33, 4849 (2000); A. Giusti-Suzor, J. Phys. B: At. Mol. Opt. Phys. **13**, 3867 (1980)] to compute cross sections and rate coefficients of low energy state to state rotational transition for H_2^+. Illustrative result for inelastic collision (IC) and super elastic collision (SEC) are given and good agreement is obtained with the result of [A. Faure and J. Tennyson, MNRAS **325**, 443 (2001)]. Cross sections are available for excitation $(N_i^+ \rightarrow N_i^+ + 2)$ $(N_i^+ = 0 - 8)$ and de-excitation $(N_i^+ \rightarrow N_i^+ - 2)$ $(N_i^+ = 2 - 10)$ for electronic energy from 10^{-5} to 0.3 eV. Results are shown in the poster.

Yves Ferro, Université de Provence Laboratoire Physique des Interactions Ioniques et Moléculaires, Marseille, France: *Interaction of beryllium atoms, dimers and Be_n clusters with graphite*. (Joint work with N. Fernandez and A. Allouche (Marseille) and Ch. Linsmeier (IPP Garching).) The interaction of beryllium atoms, dimers and clusters with graphite is studied using a DFT approach and the Quantum Espresso code package. Objectives are to study the formation of mixed Be/C materials in ITER and the modification of electronic properties of graphite and of chemical reactivity of the material.

Reetesh Kumar Gangwar, Department of Physics, Indian Institute of Technology, Roorkee, India: *Electron impact excitation and its application to plasma modeling*. (Joint work with Prof R. Srivastava (Ph.D supervisor), Dr L. Sharma and Prof A. D. Stauffer.) In low temperature plasma electron impact processes play a dominant role and reliable plasma modeling requires accurate electron impact cross section data for the various fine structure transitions considered in the model. In the light of plasma modeling we have published cross section for various fine-structure transitions from ground as well as the next excited metastable and resonance levels to the higher lying manifolds. These cross sections are obtained by using fully relativistic distorted wave theory. We have also provided analytic fits to our cross section so that these can be easily implemented in the plasma models. In the present work these cross section data are used to develop the collisional radiative (CR) model for Ar and Kr low temperature plasma. The population of 1s and 2p fine structure levels is calculated as a function of the electron temperature and electron density. The results are in good agreement with recent optical emission spectroscopy measurements. Further, for Ar plasma the intensities for 750.38 nm ($2p_1 \rightarrow 1s_2$) and 696.54 nm ($2p_2 \rightarrow 1s_5$) lines are calculated as a function of input electromagnetic power and are found to be in very good agreement with recently reported measurements of Palmero et al. It is seen that by using detailed theoretical fine-structure cross sections one can improve the CR model and hence the further applications based on the model.

Pooja Gulati, Plasma Devices Technology, Central Electronics Engineering Research Institute, Pilani, India: *Analysis of discharge parameters and spectroscopic diagnostic of DBDs*. (Ph.D. research in the group of Dr. R. Prakash.) This is a combined experimental and modelling study of the volume discharge configuration of dielectric barrier discharges filled with inert gas. An equivalent electrical circuit is created for the discharge and the spectroscopy is modelled with use of a collisional-radiative model and the ADAS codes. Suitable sets of line ratios in He I are identified and used to diagnose electron temperature and density. A particle-in-cell code is used to simulate the discharge.

Dhanoj Gupta, Dept. of Applied Physics, Indian School of Mines, Dhanbad, India: *Total ionization cross sections for Sr, Y, Ru, Pd and Ag atoms by electron impact* (joint work with R. Naghma and B. K. Antony). We have performed initial calculation of electron impact total inelastic and ionization cross section for Sr, Y, Ru, Pd and Ag atoms using spherical complex optical potential (SCOP) and complex scattering potential-ionization contribution methods (CSP-ic) respectively. The complex optical potential model is formulated from the target parameters and the atomic charge densities. The spherical charge densities are in turn derived from the Roothaan-Hartree-Fock wavefunctions defining the atomic orbital of the target. In the present study we have computed cross section in the energy range from ionization threshold to 2000 eV. These results are compared with other theories and measurements wherever available and were found to be quite consistent and uniform. In general, present data shows an overall agreement with other results.

Lars Lewerentz, Institute for Physics, Ernst-Moritz-Arndt University, Greifswald, Germany: *Particle-in-Cell (PIC) simulation of magnetic reconnection* (Ph.D. research supervised by Profs R. Schneider and R. Sydora). Driven magnetic reconnection is investigated via a gyrokinetic PIC

simulation using a code developed by Richard Sydora. The code is adapted to model the environment of the VINETA experiment at the Max-Planck-Institut für Plasmaphysik (IPP) Greifswald. This allows to compare calculations with experimental results directly. In this work the influence of boundary conditions on the diffusion layer and its current channel will be of special interest. For this a logical sheath boundary will be implemented.

Sébastien Niyonzima, Université du Burundi, Faculté des Sciences, Département de Physique, Bujumbura, Burundi: *Elementary processes in BeH^+ molecular plasma* (joint work with F. Lique, K. Chakrabarti, Å. Larson and I. F. Schneider**)**. We report a theoretical study of dissociative recombination and vibrational excitation of BeH^+ by low energy electron impact, using previously computed molecular data [J. B. Roos, M. Larsson, A. E. Orel and Å. Larson, Phys. Rev. A **80** (2009) 012501] as input for a Multichannel Quantum Defect Theory (MQDT) approach. Three electronic symmetries of BeH, $^2\Pi$, $^2\Sigma^+$, and $^2\Delta$, have been included in the calculations. We present cross sections and thermal rate coefficients in order to be used in the modelling of BeH^+ molecular ions in plasma.

Yultuz Omarbakiyeva, International Information Technology University and IETP, al-Farabi Kazakh National University, Almaty, Kazakhstan: *Cluster virial expansion for the equation of state of partially ionized hydrogen plasma*. The contribution of electron-atom interaction to the thermodynamics of partially ionized plasma has been studied using the Beth-Uhlenbeck formula [Y. A. Omarbakiyeva, C. Fortmann, G. Roepke and T. S. Ramazanov, Phys. Rev. E **82**, 026407 (2010)]. This formula makes it possible to calculate the second virial coefficient taking into account both scattering and bound states. At present the most reliable scattering phase shifts can be taken from variational calculations. Thus, for our calculations are applied phase-shifts of Schwartz [C. Schwartz. Phys. Rev. **124**, 1468 (1961)] which were obtained using trial functions that provide complete representation of the interparticle interaction. We assume the formation of bound state as H^- is possibly only at the singlet scattering channel following the analysis of the scattering length data. Binding energy for H^- is taken also from experiment. The second virial coefficient has been obtained in the range from 5×10^3 to 10^5 K using experimental data for the phase shifts and the binding energy. Going beyond the second virial coefficient, density effects such as self-energy shifts and Pauli blocking have to be considered. In particular, we have included Pauli blocking using the separable potential and have performed calculations for the density dependent second virial coefficient to cover a larger region with respect to the density. This study is a step to the systematic evaluation of the thermodynamics of partially ionized dense plasma without using artificial parameters such as a hard-core radius. The main ingredient, the systematic transition from the physical picture to a chemical one, can be obtained from a quantum statistical approach.

Houaida Oueslati, Faculty of Science of Tunis, El Manar, Tunis, Tunisia: *Multichannel quantum defect theory of $^3\Pi_u$ and $^3\Sigma_u^+$ states of H_2: rovibronic energy levels* (joint work with M. Telmini, Ch. Jungen). Theoretical study of molecular hydrogen based on multichannel quantum defect theory and the rovibronic frame transformation is presented. The results provide for the first time a fully ab initio characterization for all measured rovibronic bound level energies of the $^3\Pi_u^{+-}$, $^3\Sigma_u^+$ and $^3\Sigma_g^+$ states of H_2. The agreement with the best available experimental levels [H. M. Crosswhite, Wiley, New York (1972)] and previous theoretical calculations [S. C. Ross, Ch. Jungen, and A. Matzkin, Can. J. Phys. **79**, 561 (2001)] is good. The quantum defects are defined in a new manner [R. Gérout, Ch. Jungen, H. Oueslati, S. C. Ross and M. Telmini, Phys. Rev. A **79**, 042717 (2009)]. The quantum defect matrices thus obtained are also used to calculate the lifetimes of predissociative level c^+ $(2p\pi)$ $^3\Pi_u^+$ of H_2, the fine and hyperfine structure of the ungerade triplet states (n=2 and n=3) and the transition dipole moments in triplet states of H_2. First results are shown in the poster.

Kandasamy Ramachandran, School of Mechanical Sciences, Karunya University, Coimbatore, Tamil Nadu, India: *Modelling of plasma heating of the substrate*. Substrate heating in plasma spraying is one of the important processes that influence the microstructure of coatings and the adhesion between coating and substrate. The interaction between plasma jet and substrate is studied by a three-dimensional numerical model that predicts the temperature and velocity distributions of the plasma jet and thermal flux from the plasma to the substrate. Boundary conditions to simulate the impinging

plasma jet are obtained from the plasma arc model as well as assumed from the global mass and total enthalpy conservation relation. The effects of arc current and plasma gas flow rate on the temperature and velocity fields of the impinging plasma jet and thermal flux to the substrate are clarified. The stand-off distance strongly affects the thermal flux to the substrate. Heating rates of the steel and alumina substrates are predicted by solving transient heat conduction equation. The three-dimensional effect has a very weak influence on the substrate heating. The present model is validated by comparing the present results with previous predictions and measurements.

Daniel Romero Nieto, Molecular Simulation Engineering Laboratory, University of Trieste, Italy: *Molecular modeling of multifunctional nanostructured materials and coatings*. The project is aimed at multiscale modeling in which mesoscale dissipative particle dynamics is used to bridge the nanoscale simulated by molecular dynamics and the macroscale treated by constitutive equations and the finite element method. Application projects involve polymer-based nanocomposites and nanocoating.

Tobias Schlummer, Institute of Energy and Climate Research - Plasma Physics (IEK-4), Forschungszentrum Jülich GmbH, Jülich, Germany: *Effective rate coefficients for charge exchange recombination spectroscopy (CXRS) with fully ionized helium and argon*. (Ph.D. research supervised by Prof D. Reiter.) CXRS is an active plasma diagnostic for ion temperature, plasma velocity and impurity densities. Detailed collisional-radiative modelling of the atomic physics including beam-ion collisions, electron-ion collisions and radiative deexcitation makes it possible to use observed line ratios to determine radial profiles of T_e and T_i. CX recombination creates highly excited recombined ions that must be included in the CR model. The present work is motivated by the need to interpret CXRS emissions from argon impurity in the TEXTOR tokamak at Jülich. In order to obtain accurate line ratios it is found necessary to include principal quantum numbers up to n=20 or n=30 for direct CX influx.

Gheesa Lal Vyas, Birla Institute of Technology, Jaipur, India: *Development of Penning plasma discharge source for VUV spectrometer calibration and its characterization*. The work follows an earlier publication [Ram Prakash et al., J. Phys. B: At. Mol. Opt. Phys. **43**, 144012 (2010)] showing that a VUV spectrometer detector system can be calibrated by collisional-radiative modeling of a penning discharge source. In the present work a larger dimension penning discharge device is constructed in order to cross-check the earlier calculations. Lines and line ratios of He I in the range 350 nm – 750 nm are measured as a function of discharge conditions and are simulated in a collisional-radiative model. The pair of lines at 667.8 nm (3^1D-2^1P) and 721.3 nm (3^1S-2^1P) is recommended for an electron density measurement.

Yang Yang, Modern Physics Institute, Fudan University, Shanghai, China: *Measurements of the electron beam density in Shanghai EBIT*. In this work a portable slit imaging system is developed to study the electron beam diameter and the beam profile of the Shanghai Electron Beam Ion Trap (Shanghai EBIT). Images are detected by a charge coupled device (CCD) sensitive to both X rays and longer wavelength photons (up to visible). A numerical de-convolution method that can correct the image broadening effects caused by the finite slit width was developed to analyse and reconstruct the electron beam density distribution in the EBIT. As an example of the measured beam diameter and current density, the FWHM (full width at half maximum) diameter of the electron beam at 81 keV and 120 mA is found to be 74.89 μm and the density 2.07×10^3 A/cm^2, under a magnetic field of 3 T, including all corrections.

3. Conclusion and Recommendations

The workshop 23-27 January 2012 was the 4th in a series of similar workshops organized by the A+M Data Unit in cooperation with ICTP. Earlier workshops were held in 2003 (1 week), 2006 (2 weeks) and 2009 (2 weeks). The workshop was successful and was much appreciated by lecturers and participants alike. We look forward to organizing a similar workshop again.

A few issues are worth noting with a view to a future workshop on fusion plasma modelling and related atomic, molecular and plasma-material interaction data.

1. The workshop has a unique character in bringing together young and established researchers from several communities including both users (plasma modellers) and producers of atomic, molecular and plasma-material interaction data. This character should be preserved in future similar events.

2. The workshop is most valuable for researchers beyond the Ph.D. and that is also the audience through which the workshop has the most impact on fusion plasma modelling and the production of A+M+PMI data. We should emphasize the scientific workshop aspect in all our advertising.

3. The duration of one week is serviceable, but really 2 weeks is to be preferred especially if it can be in a timeslot somewhat later in the year to have more time to advertise the event. We have four broad topics that call for some coverage: plasma modelling, atomic processes and spectroscopy, molecular processes, and plasma-material interaction. It can't be done adequately in one week.

4. We aim to attract experts in any of the main topics of the workshop, but the focus of the workshop is on the interaction between lecturers and participants from neighbouring fields. An expert in one of main topics (plasma modelling, atomic data, molecular data, plasma-material interaction) attends the workshop primarily to learn about the other fields and their interrelation and to develop contacts with experts in these other fields.

5. The workshop is intended for researchers in fusion plasma modelling or in the production of atomic, molecular or plasma-material interaction data and we need to advertise the workshop to all these communities. Relative to 2012 we should make a special effort to attract more plasma modellers.

With these points in mind we recommend to ICTP and IAEA to organize again in the near future a joint ICTP-IAEA workshop in the area of plasma modelling and related atomic, molecular and plasma-material interaction data.

Finally we again point the reader to the additional workshop materials (including lectures, short talks and posters) available on the Web; please see these ICTP and IAEA pages:

http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a11151
http://www-amdis.iaea.org/Workshops/

Appendix 1

Joint ICTP-IAEA Workshop on
Fusion Plasma Modelling Using Atomic and Molecular Data

23–27 January 2012, ICTP, Trieste, Italy

List of Participants

ORGANIZERS/DIRECTORS

Bastiaan J. Braams	International Atomic Energy Agency (IAEA), Vienna, Austria
Hyun-Kyung Chung	International Atomic Energy Agency (IAEA), Vienna, Austria
Joe Niemela	International Centre for Theoretical Physics (ICTP), Trieste, Italy

ADMINISTRATIVE SUPPORT

Doree Sauleek	International Centre for Theoretical Physics (ICTP), Trieste, Italy

LECTURERS

Alain Allouche	Université de Provence, Marseille, France
Hyun-Kyung Chung	International Atomic Energy Agency, Vienna, Austria
Paolo Giannozzi	Dipartimento di Fisica, Università di Udine, Italy
Roger Hutton	Modern Physics Institute, Fudan University, Shanghai, China
Kai Nordlund	University of Helsinki, Finland
Kaoru Ohya	The University of Tokushima, Japan
Yuri Ralchenko	National Institute of Standards and Technology, Gaithersburg, USA
Detlev Reiter	Institute of Energy and Climate Research - Plasma Physics (IEK-4), Forschungszentrum Jülich GmbH, Jülich, Germany
Mourad Telmini	LSAMA Department of Physics, Faculty of Sciences of Tunis, University of Tunis El Manar, 2092 Tunis, Tunisia
Beata Ziaja-Motyka	HASYLAB at DESY, Hamburg, Germany

PARTICIPANTS

Fatma Argoubi	Faculty Of Sciences, University of Tunis, Tunisia
Gunnar Bandelow	Max-Planck-Institut für Plasmaphysik Teilinstitut Greifswald, Germany
Muhammad Abbas Bari	Pakistan Atomic Energy Commission, Islamabad, Pakistan
Zeyneb Bedrane	Laboratoire de Physique Théorique, Dpt. Physique, Université de Tlemcen, Algeria
Kalyan Kumar Chakrabarti	Department of Mathematics, Scottish Church College, Kolkata, India
Joel Clementson	Lawrence Livermore National Laboratory, USA
Julia Duras	Ernst Moritz Arndt Universität Greifswald, Greifswald, Germany
Michel Douglas Epée Epée	Department of Physics, Faculty of Science, University of Douala, Douala, Cameroon
Yves Ferro	Université de Provence Laboratoire Physique des Interactions Ioniques et Moléculaires, Marseille, France
Reetesh Kumar Gangwar	Department of Physics, Indian Institute of Technology Roorkee, India
Pooja Gulati	Plasma Devices Technology Group, Central Electronics Engineering Research Institute, Pilani, India

Appendix 2

Joint ICTP-IAEA Workshop on
Fusion Plasma Modelling Using Atomic and Molecular Data

23–27 January 2012, ICTP, Trieste, Italy

Agenda

Monday 23 January

08:30 - 09:00 Registration and Administrative Formalities
09:00 - 09:15 **Bas Braams:** Welcome and Introductions
09:15 - 10:00 **Detlev Reiter:** Introduction to edge plasma modelling

10:00 - 10:30 *Coffee Break*

10:30 - 11:15 **Kaoru Ohya:** Introduction to impurity transport modelling and plasma-wall interaction
11:15 - 12:00 **Mourad Telmini:** Introduction to computations for electron-molecule collisions

12:00 - 13:30 *Lunch Break*

13:30 - 13:45 **Joe Niemela:** Overview of the International Centre for Theoretical Physics
13:45 - 14:30 **Yuri Ralchenko:** Introduction to atomic data and spectroscopy
14:30 - 15:15 **Hyun-Kyung Chung:** Introduction to collisional-radiative modelling of atomic processes

15:15 - 15:45 *Coffee Break*

15:45 - 16:30 **Yaming Zou:** Introduction to electron beam ion trap experiments (talk presented by Roger Hutton)
16:30 - 17:15 **Beata Ziaja-Motyka:** Introduction to uses of atomic data for modelling warm dense matter

Tuesday 24 January

08:30 - 09:15 **Alain Allouche:** Introduction to density-functional theory modelling of fusion materials exposed to plasma
09:15 - 10:00 **Kai Nordlund:** Introduction to molecular dynamics modelling for plasma-wall interaction

10:00 - 10:30 *Coffee Break*

10:30 - 12:00 **Beata Ziaja-Motyka:** Further modelling of warm dense matter

12:00 - 13:30 *Lunch Break*

13:30 - 15:00 Participant short talks, introductions to the poster session

15:00 - 15:30 *Coffee Break*

15:30 - 17:00 Poster Session (posters will remain up on Wednesday and Thursday)

18:00 - 20:00 *Welcome Reception*

Wednesday 25 January

08:30 - 10:00 **Kai Nordlund:** Further molecular dynamics modelling for plasma-wall interaction

10:00 - 10:30 *Coffee Break*

10:30 - 12:00 **Yuri Ralchenko:** Further on atomic collisions and spectroscopy

12:00 - 13:30 *Lunch Break*

13:30 - 14:15 **Yaming Zou:** Dielectronic recombination studies using EBIT (talk presented by Roger Hutton)

14:15 - 14:45 **Roger Hutton:** Spectroscopy on EBITs

14:45 - 15:15 **Joel Clementson:** Interpretation of EBIT data; the case of tungsten

Thursday 26 January

08:30 - 10:00 **Mourad Telmini:** Further on electron-molecule collisions

10:00 - 10:30 Coffee Break

10:30 - 12:00 **Detlev Reiter:** Further on modelling with use of hydrogen kinetics database

12:00 - 13:30 *Lunch Break*

13:30 - 15:00 **Kaoru Ohya:** Further on kinetic modelling of near-wall plasma

15:00 - 15:30 *Coffee Break*

15:30 - 17:00 **Paolo Giannozzi:** Quantum simulations of materials using Quantum ESPRESSO

Friday 27 January

08:30 - 10:00 **Yuri Ralchenko:** Further on atomic physics and spectroscopy

10:00 - 10:30 *Coffee Break*

10:30 - 12:00 **Hyun-Kyung Chung:** Collisional-radiative modelling using FLYCHK

12:00 - 13:30 Lunch Break

13:30 - 15:00 **Detlev Reiter:** Further on edge plasma modelling and molecular data

15:00 - 15:30 *Coffee Break*

15:30 *Workshop closing*

Joint ICTP-IAEA Workshop on
Fusion Plasma Modelling Using Atomic and Molecular Data

23–27 January 2012, ICTP, Trieste, Italy

Participants' Short Talks and Poster

Fatma Argoubi: *Ab-initio computation of excited states of molecular hydrogen: Halfium model*.
Gunnar Bandelow: *Simulations of low-temperature plasmas.*
Muhammad Abbas Bari: *Calculation of radiative properties of hot dense plasmas.*
Zeyneb Bedrane: *How anisotropic electrons influence the density diagnostic of hot plasma*?
Bastiaan Braams: *Work of the IAEA A+M Data Unit on atomic, molecular and plasma-surface interaction data for fusion*.
Kalyan Kumar Chakrabarti: *Dissociative recombination and excitation in* H_2^+, HD^+ *and* BeH^+.
Julia Duras: *Particle simulation of ion thrusters*.
Michel Douglas Epée Epée: *Rotational transitions induced by collisions of* H_2^+ *ions with low energy electrons*.
Yves Ferro: *Interaction of beryllium atoms, dimers and* Be_n *clusters with graphite*.
Reetesh Kumar Gangwar: *Electron impact excitation and its application to plasma modeling*.
Pooja Gulati: *Analysis of discharge parameters and spectroscopic diagnostic of DBDs*.
Dhanoj Gupta: *Total ionization cross sections for Sr, Y, Ru, Pd and Ag atoms by electron impact*.
Lars Lewerentz: *Particle-in-Cell simulation of magnetic reconnection*.
Sébastien Niyonzima: *Elementary processes in* BeH^+ *molecular plasma*.
Yultuz Omarbakiyeva: *Cluster virial expansion for the equation of state of partially ionized hydrogen plasma*.
Houaida Oueslati: *Multichannel quantum defect theory of* $^3\Pi_u$ *and* $^3\Sigma_u^+$ *states of* H_2*: rovibronic energy levels*.
Kandasamy Ramachandran: *Modelling of plasma heating of the substrate*.
Daniel Romero Nieto: *Molecular modeling of multifunctional nanostructured materials and coatings*.
Tobias Schlummer: *Effective rate coefficients for charge exchange recombination spectroscopy with fully ionized helium and argon*.
Gheesa Lal Vyas: *Development of Penning plasma discharge source for VUV spectrometer calibration and its characterization*.
Yang Yang: *Measurements of the electron beam density in Shanghai EBIT*.

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