

# **27th Meeting of the Atomic and Molecular Data Centres Network (DCN27)**

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## **Book of Abstracts**



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**Discussion: Atomic uncertainties and their effect on plasma models**

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**Experiments and simulations of neon seeded radiative divertor in EAST**

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Power exhaust will be a critical issue for EAST and future tokamak devices with high heating power. Seeding the noble extrinsic impurities to increase the radiation in divertor and Scrape-Off Layer (SOL) regions through ionizations and charge exchanges, namely realizing the radiative divertor plasma operation, can effectively mitigate the high particle and heat fluxes and promote the divertor detachment to avoid overheating of the targets. To systematically investigate the behavior of Neon injection for power exhaust, both experimental and numerical simulation studies have been carried out on EAST during the past years.

Ne/D<sub>2</sub> mixture with different ratios was seeded from the divertor region as the radiators, and the divertor plasma detachment and the reduction of the heat flux on the targets can be achieved effectively as a result. Different gas puffing methods have also been investigated. Based on the experiences of different proportions and different injection methods, we successfully realized the feedback control of the total radiation power and the electron temperature near the strike point on the target with the simultaneous Ne seeding from the divertor gas puff inlet and midplane SMBI. Tungsten sputtering was also investigated during the neon seeding experiments. By using the lower Ne impurity ratio mixture with divertor detachment operation and better wall conditioning, the sputtering of tungsten could be suppressed greatly.

The Ne seeded radiative divertor experiments in EAST were also validated by SOLPS modeling. The simulation results basically agreed well with the experiments which show that Ne have relatively good performance in reducing particle fluxes and heat load on targets. Although the simulated mid-plane plasma parameters perfectly matched the experimental results greatly, it is still difficult to

match parameters well on both targets when ignoring drifts. Through reconstruction of radiation distribution by SOLPS code, most of the radiation caused by Ne impurity distributed in the region inside the separatrix in agreement with the AXUV measurements. On one hand, the above experimental and simulation results could extend our understandings of impurity seeding scenarios and underlying physics. More importantly, reasonable predictions of impurity seeding regimes in future devices, such as ITER and CFETR, can be deduced from these studies.

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## Collisional-radiative modeling for H/D plasmas and S/XB ratio for measuring W sputtering yield

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We report our recent works on collisional-radiative modeling (CRM) for H/D plasmas and  $S/XB$  ratio analysis for measuring W sputtering yield in KAERI plasma beam irradiation facility (KPBIF). The KPBIF was constructed and has been developed for simulating heat and particle fluxes in divertor plasma by adopting the concept of applied field-magnetoplasma dynamic (AF-MPD) thruster [1].

We have developed CRM for low temperature and density which solves nonlinear steady-state balance equations including processes such as radiation trapping and heavy particle collisions self-consistently [2,3]. The CRM has been applied to H/D plasmas in the electron temperature range of 2 – 7 eV and the electron density range of  $10^{11} - 10^{13} \text{ cm}^{-3}$  which are relevant to present KPBIF conditions [4]. Particular attention has been paid to investigating sensitivities of line spectra intensities and densities of particles to used atomic and molecular data in the CRM. We used actual D reaction data for electron collision of  $D_2$  molecule [5,6] as well as  $D_2^+$  molecular ion collision of  $D_2$  molecule [4], while some modelers used to replace e– $H_2$  data for D plasma assuming the e– $D_2$  data is very similar to e– $H_2$  data.

$S/XB$  ratio for determine sputtering yield of W I [7] has been measured in KPBIF and analysed by modelling using various atomic data on electron impact ionization/excitation and radiative decay. The details on available data and data needs for improving the analysis will be discussed.

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## Charge exchange cross sections in nitrogen ions and hydrogen collisions

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Impurity ions are deliberately injected into fusion plasmas for several reasons: for diagnosis using the photon emission spectra of light impurity ions, to redistribute the power transported from the plasma core to the reactor wall and to improve the control of the plasma. In order to interpret and predict the behaviour and properties of impurities in fusion plasma, a significant amount of data on the collisional-radiative characteristics of the impurities and their environment is required.

In this context, we plan to compute the cross sections for charge exchange between nitrogen ions and hydrogen atoms. Ions in ground and metastable electronic states and a broad range of collision energies (from 1 eV/u to 100 keV/u) will be considered. The different charge states of nitrogen, especially N II and N III ions, will be investigated. The outcome of our project is a complete and consistent set of cross sections that can be used in modelling fusion plasmas:

1. State-resolved cross-sections for  $N^{2+} - H$
2. State-resolved cross-sections for  $N^{3+} - H$  and  $N^{2+*} - H$
3. State-resolved cross-sections for  $N^{3+*} - H$

In order to obtain accurate cross sections for charge exchange between nitrogen ions and hydrogen atoms in a wide range of collision energies, we will employ several theoretical approaches: the semi classical and quantum Molecular Orbital Close Coupling (MOCC) at low collision energies and the Asymptotic States Close Coupling (ASCC) at high collision energies. The Landau-Zener Surface Hopping (LZSH) approach will be used to bridge between the low and high collision energy ranges.

During the talk, I will first discuss the motivation of this project, and in particular why we will focus on nitrogen ions and hydrogen collisions. The workplan, in terms of systems, schedule and employed theoretical approaches, will then be presented. After this introduction, I will shortly describe the straight-line impact parameter method (IPM) which will be used to compute cross sections for electronic processes in ion-atom collisions in the collision energy range going from 1 keV/u to 100 keV/u. After introducing the IPM, our implementation will be presented in details.

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## **Finding Key Diagnostic Lines for Divertor Molecular Dynamics based on Principal Component Analysis for Emission Spectral Dataset**

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Atomic and molecular reaction dynamics must be understood and controlled to realize efficient conversion of diverted heat load from fusion core plasmas to radiation. However, the current knowledge of the reaction dynamics is still insufficient. For example, experimentally observed radiated power in divertors is not explained by even the most advanced simulation codes. The challenge in understanding the atomic / molecular effects in the divertor is in their inherent complexity: many molecular species are involved and they interact with each other in a nonlinear manner. Exacerbating the complexities in the reaction paths, experimentally accessible quantities are very limited; analysis methods have been explored for only a few emission intensities of the atomic Balmer series and for



limited molecular lines, such as Fulcher band. Although there are many emission lines from other excited states of hydrogenic and other impurity molecules, their analysis methods have not been established and thus they have been rarely measured.

In this work, in order to find unexplored features in molecular emission spectrum, a principal component analysis (PCA) is applied to high-definition spectra covering the entire visible range with 0.1 nm wavelength resolution, that are taken for 16 different experiment from the LHD divertor regions (totalling 150 frames). PCA approximates all the observed spectra by a sum of a few orthogonal bases. When the spectra are observed for variety of plasma conditions, emission lines that have different parameter-dependencies are categorized into different bases.

We found that most of the hydrogen molecular lines are categorized into a single basis, while a few distinct lines emerge in another basis. After the deeper examination, it is found that the lines extracted from PCA are H<sub>2</sub> emission lines from the EF<sup>1</sup>Σ<sub>g</sub> state and their distinct behavior is characterized by the long radiative lifetime of the state (~102 ns). As the population influx and outflux of this state are dominated by electron-impact transitions, the  $n_e$  dependence on the population is cancelled out. On the other hand, the intensity of typical emission lines is nearly proportional to the electron density as the spontaneous radiation determines the lifetime of their upper states (e.g., ~100 ns for D<sup>1</sup>Π<sub>u</sub> state).

This finding leads to new diagnostic insights of the molecular reaction dynamics: the ratio of the two emission lines can be used to diagnose  $n_e$  at the emission location, and the line intensity from the EF<sup>1</sup>Σ<sub>g</sub> state can be used to infer the molecular density. A simplified collisional-radiative model is constructed from the electron-impact cross sections and spontaneous transition rates related to these states, which reveals a nearly linear  $n_e$ -dependence of the line ratio and insensitivity on  $T_e$ . We constructed a simple collisional-radiative model and estimate  $n_e$  at the emission location (which is close to the divertor plate). This shows a strong correlation with ~3 times smaller than the value of  $n_e$  measured independently on the last closed flux surface (LCFS). This correlation is consistent with previous studies.

In this work, the use of a pattern-recognition technique has been demonstrated to find underlying physics embedded in the complex spectra. This finding is not only useful for reaction studies in divertors, but also suggests the effectiveness of the approach. Application of a similar method to other parameter spaces, such as the high-density detached divertor in tokamaks and MPEX plasmas may reveal information more relevant to fusion power plant divertors.

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## Electron impact ionization for $\text{N}^+$ and $\text{N}^{2+}$ ions

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Electron impact ionization and recombination define charge state distribution in collisional plasma. Line intensities in the spectra from plasma strongly depend on the population of ions.

The aim of this work is to study electron impact ionization from the ground configuration levels of N<sup>+</sup> and N<sup>2+</sup> ions. The study includes both direct and indirect ionization processes. The indirect process is investigated as excitation to autoionizing states, followed by Auger transitions.

The Flexible Atomic Code (FAC) [1] is used to calculate energy levels, radiative and Auger transition probabilities, electron-impact ionization, and excitation cross sections. The ionization and excitation cross sections are investigated in the distorted wave (DW) approximation. The DW cross sections are estimated in the potential of the ionizing ion.

The study includes direct ionization from the  $2\sigma$  and  $2\pi$  subshells of the ions. The direct process contributes to  $\sim 90\%$  and  $\sim 80\%$  of the total ionization cross sections for the  $N^+$  and  $N^{2+}$  ions, respectively. The scaled DW cross sections have to be used to explain measurements [2, 3] for the  $N^+$  ion.

The DW cross sections obtained for the ground configuration levels of the  $N^{2+}$  ion show good agreement with experimental data. It should be noted that the three lowest energy levels of the 222 configuration have lifetimes lower than  $\sim 10^{-3}$  s. These levels can also contribute to the experimental data [4]. The EA channels corresponding to excitations from the  $2\sigma$  and  $2\pi$  subshells are included in the study for the 222 configuration of the  $N^{2+}$  ion. Excitations up to shells with  $n = 20$  are considered for the indirect process. The study shows that the excitations from the  $2\sigma$  subshell provide a similar contribution to the excitations from the  $2\pi$  subshell. It should be noted that the EA channels corresponding to excitations from the  $2\sigma$  subshell converge more slowly compared to the excitations from the  $2\pi$  subshell.

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## Measurement of Ion impact X ray Emission by a novel technique based on High pressure Gas Ampoules in Silicon Blisters

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Measuring X-ray production cross sections of noble gases by proton impact is always a challenge, due to the low intensity of photons produced in a low-density environment. Our proposal is to avoid this disadvantage by employing a novel technique which measures these cross sections on highly stable high-density-pressure gas ampoules implanted in the crystalline structure of Si. These blisters are covered by thin layers of a few nm of Si, which prove to be very stable, even decades after their manufacturing date. The atoms can be contained in gaseous form with pressures estimated in values as high as 3 GPa. By irradiating these samples with protons, an x-ray signal can be measured with a SDD detector. This means that under these conditions the blisters can be used as a thin sample for x-ray production cross section measurement, provided that their gas density is known. To obtain a good estimation for this quantity, the samples are analysed with different techniques, namely, RBS, XPS and AFM. Finally, using a Tandem Ion Accelerator, K-shell x-ray productions cross section is measured from characteristic line yields produced by proton impact with energies ranging from 0.2 to 3.4 MeV. The results obtained in this work might be the first stage in developing a reliable method for the measurement of cross sections in noble gases (Ar, Kr, Xe, ...). Furthermore, we proposed to extend the analysis to different substrates, as graphite, to carry out the cross-section measurement in the best conditions available, i.e., with the optimal blister size, pressure and substrate that produces the least interference during the X-ray detection. It should be noted that the resulting cross sections should be equivalent to low-density gaseous target measurements because, even in high-pressure ampoules with densities typical of a solid, the confined gas is only a few nanometres thick, so that the single collision condition remains valid.

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## **Application of Neural Networks for determining Stopping Powers**

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