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Nitrogen retention in ASDEX Upgrade

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Abstract

We investigated the transport of nitrogen through the plasma and the interaction of nitrogen with tungsten under divertor exposure conditions during nitrogen-seeding experiments in ASDEX Upgrade. Using the divertor manipulator system, tungsten samples were exposed to well-characterised L-mode plasmas with and without nitrogen seeding. We also simulated nitrogen transport and re-distribution in these discharges by self-consistent WallDYN-DIVIMP modeling. For these simulations we applied a W-N surface model based on laboratory experiments and plasma backgrounds from SOLPS. In contrast to the conclusion from Ref. [5] we find that the N retention in ASDEX Upgrade is in agreement with results from laboratory experiments.

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1. Introduction

The migration of impurities is a key process in the area of plasma-surface interaction, as it controls net erosion, material mixing, plasma contamination and tritium retention [1, 2]. Nitrogen (N) is a convenient choice for migration studies for several reasons: First, it is tolerated by the plasma and easy to handle and to detect. In addition, the migration of N is of interest for power exhaust studies, where N is used to control the divertor target heat load.

Nitrogen is special in its interaction with metal walls. Different from hydrogen or noble gases, N is retained in the walls by forming compounds such as tungsten nitrides [3]. On the other hand, N does not form layers on top of the original wall material and the diffusion of N in tungsten is negligible below 800 K [4]. Thus, the N wall content saturates and further N influx is reemitted from the surface. N retention and release have been studied in laboratory and tokamak experiments. From laboratory experiments, where pure N has been implanted into polished samples, and accompanying modeling, a saturation areal density of about $1 \cdot 10^{20}$ N/m^2 was determined for walls at temperatures below 500 K [4].

Three different ideas to study the latency of N in ASDEX Upgrade (AUG) have been followed in the past: In Ref. [5] a model has been developed to feedback control the N puff for radiative cooling in AUG. The results from Ref. [5] agree qualitatively with the laboratory experiments. However, the N saturation areal density deduced from this model is a factor of ten larger than the one found in laboratory experiments. As an explanation for this increased N retention Ref. [5] suggested the roughness of the AUG wall tiles. In

Ref. [6] residual gas analysis confirmed the retention of N in AUG and demonstrated that part of the injected N_2 is converted into ammonia. Ammonia adsorbed to the walls is only slowly released, so ammonia formation could also contribute to the observed N latency. In Ref. [7], ^{15}N was injected into AUG from the low field side before a vessel opening and the ^{15}N content of a set of tungsten wall tiles was measured. This experiment revealed a highly toroidally asymmetric deposition for the chosen injection location. However, the variation in the N content was smaller than suggested by ASCOTT modeling, which did not take into account the N saturation. At the time of these experiments also C was injected into the machine. Therefore, it is likely that N+C co-deposits have formed and the measured N areal densities cannot be compared to laboratory experiments on pure W.

We performed a set of dedicated AUG experiments to investigate N migration and retention. Migration is defined by its multi step nature: The erosion of wall material by the plasma, its transport through the plasma, the re-deposition of the eroded material and its potential re-erosion [2]. To take into account all these steps and the complex plasma-wall interaction of N, our analysis is based on WallDYN simulations [8, 9].

2. Experimental set-up

The chosen plasma scenario was a well diagnosed L-mode discharge, with a magnetic configuration similar to discharge #27100 described in [10], with moderate ECRH heating of about 400 kW and a line averaged density of $4 \cdot 10^{19}$ m^{-3}.

The magnetic geometry in the divertor region is shown in Fig. 1. This figure also shows the position of the AUG divertor manipulator (DIM) system. With the DIM system samples can be exposed to single discharges and then be retrieved for ex situ analysis. The samples exposed during this study had about 2 μm thick W layers on a fine grain graphite substrate produced by combined magnetron sputtering and ion implantation [11]. This is a similar set-up as used for AUG tiles and allows to test whether N retention in this rough surface is larger than expected from laboratory studies on smooth samples. The temperature of the samples was estimated to remain below 420 K, so the temperature dependence observed in Ref. [4] does not play a role. The experiments described here were performed on two different days in discharges with the numbers #29695, #29696 and #29730 to #29732. The discharge #29695 was a reference discharge without N puff. All other discharges were seeded with N_2 as shown in the time trace in Fig. 2. To maintain toroidal symmetry valves with 8 toroidally distributed outlets in the roof baffle were chosen for the N_2 puff (see Fig. 1). This choice is also of practical relevance, as these valves are regularly used for N_2 puffing at AUG. A small average N_2 puff of $2.9 \cdot 10^{20}$ N/s was chosen. As a minimum flux is required to open the valve, a modulation of the puff (10 ms on, 30 ms off) was required. The valve is connected to the outlets in the roof baffle via a tube of 3 m length. The time required for the N_2 to move from the valve location through the tube to the outlet is above 0.1 s, so that the original modulation in the puff is smoothed out.

There were nine discharges without N-seeding prior to #29695 and there were no N_2-seeded discharges between #29697 and #29730. According to N spectroscopy and residual gas analysis, the initial background N content (N ion concentration in the core plasma about 0.2 %) was a factor of 2–7 lower than the N content during the N_2 seeded phase. The initial N background for #29695 and #29696 was slightly higher than the

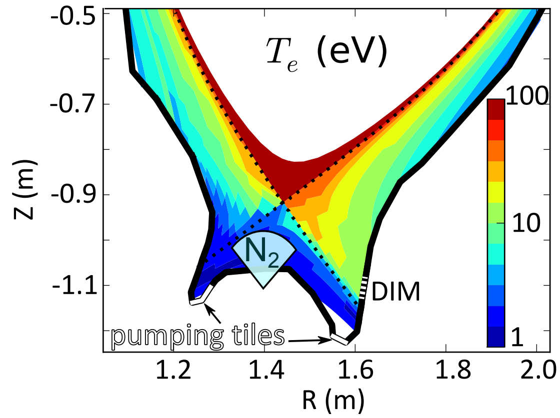

Figure 1: Position of N valve, divertor manipulator (DIM) (dashed region) and pumping tiles used in WallDYN to mimic pumping by the vacuum system; T_e plasma background for N seeded phase.

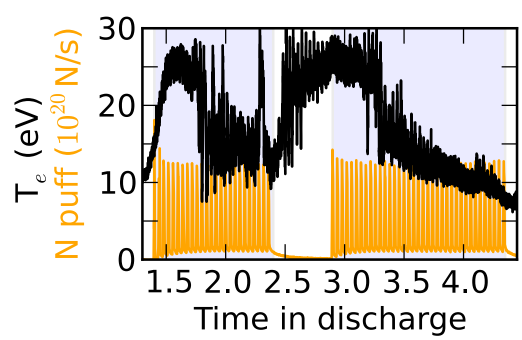

Figure 2: N_2 puff (lower curve) and electron temperature close to the outer strike point during discharge #29696.

initial N background in #29730.

Despite the low N_2 seeding rate, the N_2 puff induced a transition into the fluctuating detachment state [10]. The accompanying drop in the electron temperature close to the outer strike point is shown in Fig. 2. During the unseeded phase in the middle of the discharge the plasma N content drops and the divertor plasma changes back to its original (higher T_e) state. Due to the legacy of N in AUG the background N level rises during our discharges and the low T_e phases become longer.

To determine the amount of nitrogen in a sample after exposure with the DIM, we used nuclear reaction analysis (NRA). The protons resulting from the nuclear reaction $^{14}\mathrm{N}\,(^{4}\mathrm{He},{}^{1}\mathrm{H})\,^{17}\mathrm{O}$ were counted at a scattering angle of 135°. An energy of 4940 keV was chosen to optimise the signal from nuclear reactions with N over the background. The number of counts was converted into the N areal density by comparison to the signal generated by a CN_x layer, whose N areal density is known from Rutherford backscattering measurements. Also protons emerging from a nuclear reaction with boron were recorded and quantified by comparison to a calibration sample.

3. WallDYN modeling of N transport and retention

To support the interpretation of the experiments we performed simulations with WallDYN-DIVIMP [8, 9] a self-consistent global erosion-deposition model. This model simulates the evolution of the surface composition of the first wall, which is discretised for this purpose into 59 poloidally distributed wall tiles. The size of each wall tiles is adapted to the local conditions, with a small poloidal extent in the divertor and larger tiles at the main wall. An important input for WallDYN and DIVIMP is the plasma background, i.e. spatially resolved data on the plasma density, temperature and flow velocity. The plasma background is used in our simulations to calculate the energy of ions impinging on the walls, to extract D fluxes onto the walls and to calculate with DIVIMP [12] a matrix describing the re-distribution of impurities [8]. For our simulations we used plasma backgrounds generated with the SOLPS5.0 code package [13]. As the SOLPS solution only covers the part of the Scrape-off layer (SOL) directly connected to both divertors via magnetic field lines, we used an onion-skin model (OSM) [14] to extrapolate this solution up to the main wall. The electron temperatures from the N-seeded plasma background are shown in Fig. 1.

As the divertor plasma switches between two states depending on the N content of the plasma (see section 2) we also used two plasma backgrounds. The first one corresponds to the plasma state without N puff. The second solution includes the effect of an N puff on the plasma, reproducing to the cooler outer divertor conditions. This regime occurred in our experiments from about 1.7 s to 2.5 s and from 3.3 s to the end of the discharge.

In DIVIMP simulations the impurities are launched as atoms with an energy of about 3 eV. In reality, nitrogen coming directly from the puff (and maybe nitrogen recycling at saturated surfaces) enters the plasma in the form of thermal N_2 molecules. However, in SOLPS simulations only a small difference was found between using N atoms and N_2 molecules [15]. The most likely effect of molecules would be to change the spatial ionization pattern in comparison to N atoms. To test the sensitivity of the WallDYN simulations to the ionization pattern we varied the initial energy of the N atoms (from around 0.03 eV to around 30 eV). The predicted deposition pattern in the outer divertor did not change within this range of initial energies.

The transport of particles perpendicular to the magnetic field lines is modeled in DIVIMP via an anomalous diffusion coefficient, which is constant over the whole computational domain. We used a diffusion coefficient of $D_\perp = 0.5\ m^2s^{-1}$. This is the value of the particle diffusion coefficient used in the SOLPS simulation of the background plasma close to the separatrix. A comparison with a simulation based on a re-distribution matrix calculated with $D_\perp = 1\ m^2s^{-1}$ resulted in the same outer divertor N deposition.

To set up a self-consistent set of equations for the evolution of the surface composition and the impurity fluxes, a description of the implantation and erosion processes is required. The original model implemented in WallDYN is suited for elements which can accumulate on the surface. We extended the model to mimic the saturation of a species at a given atomic concentration in the reaction zone (see Ref. [8]). Ref. [4] suggests a maximum concentration of 50 % for N in W. However, WallDYN averages the concentration over the reaction zone thickness of 4 nm (corresponding to the typical implantation depth). The SDTrimSP simulations in Ref. [4] show that the concentration of 50 % is only reached in part of the corresponding volume. Therefore, the maximum concentration in WallDYN was adjusted to reproduce the value of $1 \cdot 10^{20}$ N/m^2, suggested as mean saturation areal density in Ref. [4]. The N areal density may still rise above this value when N is co-deposited with boron or tungsten.

To mimic the pumping of N_2 by the vacuum system we specified wall tiles (white regions in Fig. 1) where sputter and reflection yields are zero.

Due to regular boronisations, parts of the AUG first wall are covered with boron. Boron, like tungsten, forms a stable compound with N. Furthermore the formation of BN can be described in the binary collision approximation, neglecting chemical effects such as

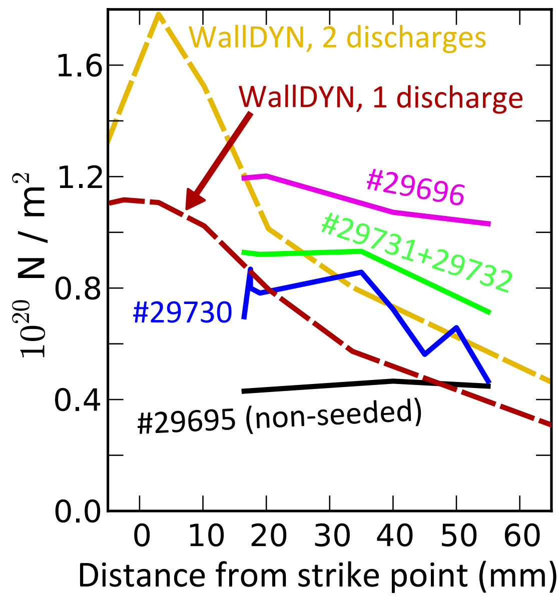

Figure 3: N content measured in divertor manipulator samples (solid line, discharges are described in section 2) and WallDYN simulation results (dashed line).

thermal diffusion [17], so the WallDYN model for the saturation is also applied for boron containing regions of the wall.

4. Results and discussion

4.1. Divertor manipulator N deposition

The N areal densities measured in the samples exposed to AUG discharges are shown in Fig. 3. This figure also shows, cropped to the outer divertor region, the N areal density predicted by WallDYN. The lowest N content can be found in the sample exposed to the non-seeded discharge. SDTrimSP simulations [16] based on an estimate for the (residual) N flux from spectroscopic measurements predict a comparable N areal density of $0.3 \cdot 10^{20}$ N/m^2.

The N content of the samples exposed to one N-seeded discharge is higher than the one exposed to the unseeded discharge. However, the sample exposed to #29696 has a notably larger N content than the sample exposed to the nominally identical discharge #29730. The N content from the sample exposed to #29731 and #29732 is located between the samples exposed to #29730 or #29696.

One conclusion from this is that there is no obvious fluence dependence, i.e. no factor two increase of the N content in the sample exposed to two discharges and only a marginal decrease over the sample length away from the strike point. This result is reproduced by the simulation, where there is only a little increase in the N content from one to two discharges. Another conclusion is that the saturation areal density of the rough samples exposed to AUG is comparable to the areal density determined for smooth surfaces in laboratory experiments and SDTrimSP simulations. This indicates that N ions can only reach parts of the surface not shadowed by a protruding surface structure [18].

A remaining question is why the N content in the sample exposed to #29696 is larger than in the other samples. Spectroscopic measurements show that the plasma N content in #29696 was larger than in #29730 and comparable to #29732. A complicating feature is that a higher plasma N concentration can lead to different plasma conditions. Especially the change in the electron temperature can modify the N content in the samples by changing the N ionization pattern, the temperature gradient force, re-erosion and implantation energy and angle. It should also be noted that the steady state N content under D-N bombardment can decrease with an increasing N fraction in the incoming flux [4].

The boron content of the sample exposed to #29696 was also larger than in the sample exposed to #29730 and comparable to the boron content of the sample exposed to #29731 and #29732. The boron areal densities in the samples were $0.3–0.7 \cdot 10^{20}$ B/m^2, so that co-deposition of N with B could play a role. The similar areal densities of N and B reflect their similar presence in the plasma (B content is typically around 1 %). Although the lack of a definite explanation is not fully satisfactory, one has to conclude that the variation observed between #29696 and #29730 indicates the limit of accuracy which could be reached in the present experiments.

Finally we want to note that the N content of the sample exposed to #29696 was measured a second time half a year after the first measurement and had not changed during this time.

4.2. Total N retention in AUG

The presented measurements show that the N content in samples with a rough surface is not higher than expected from laboratory experiments on smooth samples. This raises the question on what causes the discrepancy in the N saturation areal densities measured by surface analysis and deduced previously from the feedback model for N seeding in AUG [5]. As already mentioned, the N saturation areal density given in Ref. [5] is based on a model used to feedback control N seeding in AUG. For this model the plasma wetted area in AUG was estimated to 3.5 m^2. The saturation areal density was then treated as fit parameter and a value of 10^{21} N/m^2 was applied to reproduce the measured temporal evolution of the nitrogen flux. However, the physical quantity measured by the model is rather the a storage capacity of AUG, $3.5 \cdot 10^{21}$ N atoms, than the areal density.

The number of N atoms stored in AUG can also be estimated with WallDYN. WallDYN self-consistently simulates the N fluxes and resulting N areal densities on the complete first wall, without the need to manually specify a plasma wetted area. The N areal densities are calculated in WallDYN by a model including reflection, physical sputtering

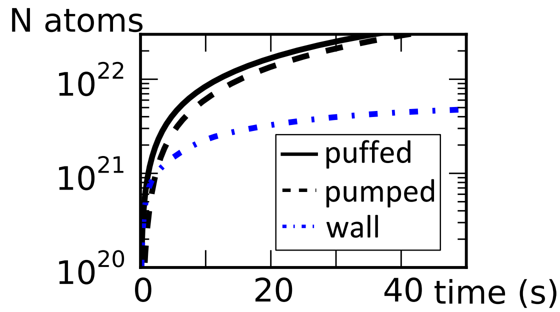

Figure 4: WallDYN simulation on the long term N retention in AUG: Number of puffed N atoms (solid line), pumped atoms (dashed) and wall content (dash-dotted)

and saturation at an N areal density of about $1 \cdot 10^{20}$ N/m^2. The predicted number of N atoms retained in the first wall of AUG is shown in Fig. 4. This simulation used the N-seeded plasma background, the rather conservative diffusion coefficient of $D_\perp = 0.5$ m^{2}s^{-1} and a constant puff ($8.6 \cdot 10^{20}$ N/s) comparable to the one used in Fig. 7 of Ref. [5].

According to this simulation, the N content in the walls of AUG saturates at about $5 \cdot 10^{21}$ N atoms. This agrees, within the uncertainty of such a calculation (caused e.g. by the toroidal asymmetry of parts of the main wall), well with the number of $3.5 \cdot 10^{21}$ N atoms from Ref. [5]. Also the fluence dependence of the number of retained N atoms is similar: The wall content for $2 \cdot 10^{21}$ puffed N atoms is $1 \cdot 10^{21}$ N atoms in WallDYN and $1.4 \cdot 10^{21}$ N atoms according to Fig. 7 of Ref. [5]. So both models predict the same number of retained N atoms, but according to WallDYN large parts of the wall contribute to the N retention. This suggests that the apparent discrepancy reported in Ref. [5] is due to an underestimation of the plasma wetted area used to calculate the areal density.

5. Conclusion

The accumulation of N in W coated samples exposed to the divertor plasma of ASDEX Upgrade has been measured with NRA and simulated with DIVIMP-WallDYN. The measured N content of samples exposed to one and two N seeded discharges is comparable, so that a steady state of the local N content must have been reached within one discharge.

Our simulations of N retention in ASDEX Upgrade based purely on established physical models give a good agreement to experimental measurements. This is a successful benchmark of WallDYN and allows to base the interpretation of the experiments on the WallDYN simulations. Beyond the results published in this article, a comparison to further diagnostics and the use of plasma backgrounds based on the OSM model allows to identify remaining weak spots in the simulations, study the physical effects underlying impurity migration, improve our understanding of ammonia production and to suggest further experiments. This work will be presented in a future publication.

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