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Abstract

Molybdenum is used as plasma-facing material in tokamaks and as material for plasma optical diagnostics mirrors. Harsh conditions of neutron irradiation, exposure to hydrogen isotopes and helium ions, and high operating temperatures result in degradation of molybdenum surface and ultimately limit their lifetime in a fusion power plant. In the current paper, intake and subsequent thermal release of deuterium from self-irradiated by high energy (1 MeV) ions molybdenum as a function of irradiation dose are investigated. Several characteristic temperature regions where deuterium release takes place are identified and attributed to trapping of deuterium in intrinsic and radiation-induced microstructure defects. This attribution is further validated by molecular dynamics modelling which confirms that increase and saturation of vacancy concentration found in simulations follows increase and saturation of experimentally determined deuterium content. Deuterium inventory and vacancy content saturate at a damage level of around 0.2 dpa (displacement per atom), similar to recent modelling and experimental studies of iron and tungsten. Reflectivity measurements of irradiated molybdenum show that it is only slightly affected by damage up to 1 dpa.

Keywords: thermal desorption spectrometry, reflectivity, molecular dynamics, molybdenum, hydrogen

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1. Introduction

Molybdenum was considered as a plasma-facing material from the early years of tokamak design. In particular, it was used in Alcator-C tokamak, that was able to explore plasma pressures up to 2 atm and magnetic fields approaching 8 T [1,2]. Currently, molybdenum is the first-wall material in EAST, Experimental Advanced Superconducting Tokamak [3]. Low sputtering yield of molybdenum and its ability to withstand high neutron flux, high thermal loads, and peak surface temperatures in excess of 1000 °C as a plasma-facing material [4] are comparable to that of tungsten [5], while Mo better resists radiation-induced embrittlement [6]. While currently another body-centered cubic (bcc) metal with similar properties, tungsten is preferable plasma-facing material because of its less problematic activation under exposure to divertor or blanket first-wall irradiation, adjustment of Mo isotopic composition could reduce or remove the activation problem [7]. Currently, molybdenum is a material of choice for use as a mirror in optical diagnostics systems of ITER and its successors, necessary to view the plasma in a wide wavelength range, from nanometres to hundreds of micrometres [8-12]. The conditions under which these mirrors will operate in ITER will include temperatures up to 250 °C [13,14], and the level of neutrons and plasma particles irradiation well beyond those in current tokamaks. For example, total energy throughput of 220 GJ and a divertor ion fluence of 1.8×10^{27} has been achieved in a single JET campaign between 1999 and 2001 [14]. Even higher energy throughput of 496 GJ that was achieved in three ITER-like wall campaigns in JET corresponds to around 550 ITER discharges of 400 s duration, but only to around 15 if scaled by energy input or even less than two in terms of the divertor fluence [15]. The ability of mirrors to withstand these harsh conditions for long time without changing their optical properties is necessary for successful functioning of the fusion power plant. This was a motivation to perform the studies of hydrogen intake by self-irradiated molybdenum and the influence of irradiation on its reflectivity.

Early studies of hydrogen in molybdenum dealt with trapping efficiency and saturation of hydrogen intake in Mo subjected to low-energy (up to 30 keV) hydrogen ions [17,18]. Consequently, the following thermal desorption spectrometry (TDS) studies were able to reveal low-temperature release peaks between 200 K and 600 K [18], but found no high-temperature peaks, which can only be revealed under high energy irradiation. Myers and Besenbacher [19] investigated trapping of deuterium by helium bubbles in Mo. In a study on implantation of Mo with low-energy (up to 1 keV) deuterium ions [20], a low-temperature TDS peak at 400 K and high-temperature peak at 650-700 K were attributed to ion-induced defects, while the

intermediate peak between 500 K and 600 K was ascribed to deuterium retention in natural traps. However, this attribution can only be confirmed in studies involving wide range of ion-induced damage and comparison with unirradiated samples. In this paper, for the first time results for deuterium retention obtained for molybdenum self-irradiated up to a high dose of 1 displacement per atom (dpa) by high energy (1 MeV) ions, are presented. These results are validated by molecular dynamics modelling of concentration of vacancies created in Mo as function of irradiation damage. In addition, reflectivity of irradiated molybdenum samples is investigated. In recent years, influence of irradiation of molybdenum mirrors with helium ions in the energy range up to several keV has been extensively studied [21-25], and it was found that even relatively low dose of 0.1×10^{17} ions/cm^2 results in noticeable decrease of total reflectivity [24], while at higher dose of 3×10^{17} ions/cm^2 of helium irradiation, reflectivity decreased by up to 20% [22]. At the same time, even 30 dpa dose of low-energy Mo self-irradiation resulted only in a slight decrease of reflectivity [22]. In this paper, we study reflectivity changes under irradiation by high-energy (1 MeV) Mo^+ ions with a dose up to 1 dpa.

2. Methods

2.1. Sample preparation

Pure Mo (99.97%), 1mm thick sheet was sourced from Plansee and cut using electro-discharge machining (EDM) into 8mm x 8mm samples before being annealed in vacuum for 2 hours at 1200 ˚C (Dept. of Engineering Science, University of Oxford). The samples were then polished with SiC paper up to a grit of 4000 followed by diamond suspension (8µm - 1µm) and finally colloidal silica until a mirrored surface was achieved. Some samples were irradiated at the University of Surrey's Ion Beam Centre in the 2 MV Van der Graaff accelerator with 1 MeV Mo^+ ions at room temperature. The number of created vacancies as function of depth was estimated using SRIM software [26-28], see Figure 1. Note that the SRIM calculates overall number of Frenkel pairs (vacancies and interstitials) created by bombardment, not the actual damage in the system after relaxation. Following [29], we refer to SRIM results as canonical dpa. The SRIM results can be used to estimate the number of ions (fluence) required for a specific damage level for a particular ion energy. The fluence necessary to obtain irradiation dose of approximately 1 canonical dpa in the surface layer of 200 nm by 1 MeV ions was found to be 1.05×10^{14} ion/cm^2; for lower doses, fluence was decreased accordingly. Overall,

irradiation was performed up to three damage levels of nominally 0.01, 0.1, and 1 dpa; one sample was left in a non-irradiated condition (0 dpa).

Samples irradiation levels, exposure conditions, and subsequent characterization methods are listed in Table 1. Exposures to deuterium were carried out using the Device for Exposure to Low-energy Plasma of Hydrogen Isotopes (DELPHI) – facility at the Culham Centre for Fusion Energy, and a detailed description of the device used for the experiments is given in [30]. For each experiment, a sample was mounted to the sample holder plate (Figure 2). The sample was placed into the sample loading chamber with a load lock system to allow sample handling within a vacuum of $\leq 5.0 \times 10^{-6}$ mbar. The sample is then transferred onto a sample stage mounted below a boron nitride plasma chamber, where a 2.45 GHz radially symmetric microwave field provides the main heating source for the deuterium plasma. Deuterium ions are extracted from the plasma via ion optics and guided to the sample. Experiments were carried out using a beam flux of approximately 10^{18} ions/m^2·s. Measurements of the ion species fractions were not made for this system, however measurements of ions produced in a similar way show approximately 0.97 D^+_3, 0.02 D^+_2 and 0.01 D^+ [31] suggesting an average of 2.96 deuterium atoms per incident ion. Ions are extracted using an anode set to 0.6 kV and an extractor set to -0.3 kV, providing an ion energy of 600 eV, or an average of 200 eV per deuterium atom. Low energy ions are used to prevent further ion damage to the samples. The ion current is measured via voltage drop (eV) over a small resistor to ground, with a high accuracy multimeter measuring a primary current applied to the sample stage and a secondary current applied to a shield sheet with the sample placed in the middle. The ratio of primary and secondary current can be used to calculate the beam divergence and ensure a uniform ion exposure over the sample. Exposures were carried out at ambient temperature, for a duration of ~5 hrs for each sample. The plasma performance and plasma stability are monitored during exposure by an optical light source (diode) fixed to the outside of the plasma chamber. After exposure, plasma was turned off and the sample was extracted and stored under vacuum for a fixed amount of time before TDS analysis.

2.2. Experimental

Thermal desorption spectrometry (TDS) measurements were performed at UKAEA using Hiden Analytical TPD workstation Type 640100. Details of the instrument can be found in [32]. All samples were annealed from room temperature to 1273 K at a constant ramp rate of 10 K/min and held at a maximum temperature for 1 hour. Base pressure in the measurements

was in the range of ~$2*10^{-9}$ mbar. The released gases were detected using line-of-sight quadrupole mass spectrometer; molecular fluxes of masses 3 (HD molecules) and 4 (D_2 molecules) were quantified using H_2 and D_2 calibrated leaks and used for determination of deuterium atomic release flux and total deuterium content according to the equation

$$D(atoms)=HD(molecules)+2*D_2(molecules)$$

Time delay between deuterium loading and TDS measurements was 1 day, except sample Mo41, that was measured one month after exposure to deuterium.

Reflectivity measurements were performed on samples irradiated up to several levels of damage but not exposed to deuterium and subsequent TDS: Mo3 (0.01 dpa), Mo6 (0.1 dpa), and Mo2 (1 dpa). Measurements were performed using two diode array spectrometers: getSpec-2048 in the 350-1100 nm range and getSpec-NIR1.7-256 in the 900-1700 nm range. The accuracy of the measurements is ~1%; reproducibility, i.e., results obtained on the same sample in several measurements is also ~1%.

2.3. Modelling

In order to validate experimental results on deuterium inventory as function of damage, modelling study of defect accumulation in molybdenum under irradiation has been performed. Straightforward attempt to model self-ion irradiation is hardly possible because of large penetration depth resulting from high energy of incoming ions (1 MeV). Molecular dynamics studies of systems with dimensions of the order of several thousand Angstrom (see the penetration depth in Figure 1) and, consequently, including billions of atoms are beyond current computer power. However, in the recent years several new methods have been developed that allow simulating irradiation damage without explicit modelling of ion bombardment. Chartier et al. used Frenkel pairs (vacancy – interstitial) accumulation method to study radiation resistance of pyrochlores [33] and the microstructure evolution of iron under irradiation [34]. In this method, irradiation is simulated by displacing random atoms away from their lattice positions in the supercell combined with molecular dynamics runs between such displacements. Similar method, the creation-relaxation algorithm was used by Derlet and Dudarev [29] to model accumulation of damage in iron and tungsten. They combined random atomic displacement (Frenkel pair creation) with subsequent energy minimization. Their results have shown that initially linear relationship between number of Frenkel pairs introduced and the

number of vacancies created in the system saturates at doses of the order of 0.1 to 1 canonical dpa.

To simulate experimental conditions of self-ion irradiation, the Frenkel pairs accumulation method combined with molecular dynamics runs between displacements, was chosen. The simulations were performed using LAMMPS molecular dynamics simulator [35,36] using the embedded atom method interatomic potential by Ackland and Thetford [37]. This potential is widely used for modelling mechanical properties and defect formation in molybdenum [38-41]. Cubic simulation box included 65536 Mo atoms in 32×32×32 bcc unit cells. Simulations were performed in NPT ensemble at pressure P = 0 Pa and three temperatures: T = 300 K, in agreement with irradiation conditions, and T = 600 K and T = 900 K, close to the temperature of fusion device. At each step, a Frenkel pair was created by choosing random Mo atom and randomly displacing it within the simulation box. To avoid unphysically large energies, it was checked that after the displacement, the atom was not closer than 1 Å to any other atom; in that case, displacement was repeated. After each displacement, molecular dynamics run of 1 ps was performed to ensure relaxation of temperature and pressure to their chosen values. Overall, simulation included creation of 65536 Frenkel pairs, corresponding to total canonical damage of 1 dpa.

3. Results

3.1. Experimental

TDS deuterium spectra of the samples studied are shown in Figure 3. For all irradiated samples, spectra are characterized by a prominent peak at around 550 K. In the undamaged sample (Mo7), this peak is absent, but a lower temperature peak is seen at 400-450 K. With increasing damage, the height of the 550 K peak increases sharply, so that the lower temperature peak either disappears completely, or remains as a shoulder feature. Another shoulder-like feature can be seen just above 600 K in sample Mo41 irradiated up to 1 dpa and measured after 1 month delay. Finally, the logarithmic plot (Figure 3b) reveals small broad peak at around 1100 K in all the irradiated samples. Its height, similarly to the case of main peak around 550 K, increases with the increase of irradiation dose.

Overall deuterium inventory as a function of damage is shown in Figure 4. Here the saturation of deuterium content takes place above 0.1 canonical dpa. This is similar to the case of tungsten

[42,43], where deuterium content saturation results from saturation of damage with dose. Similar results were also found recently in direct atomistic simulations of highly irradiated tungsten and iron performed using the creation-relaxation algorithm [29]. Increasing delay between the exposure and the TDS results in the decrease of the deuterium amount, as seen from the comparison of 1 dpa samples investigated one day (shown as blue dot) and one month after exposure (shown as red dot in Figure 4).

Total reflectivity as function of wavelength is shown in Figure 5. Specular reflectivity is around 90 % of the total for all samples. In almost all wavelength range 400-1600 nm, reflectivity is the same for the three samples within 1.5%, which is within measurement uncertainty. It is possible to conclude that with increasing irradiation damage, no further degradation is observed. Overall, self-ion irradiation, even up to relatively high damage of 1 dpa, hardly changes reflecting properties of molybdenum. Of course, under the realistic conditions of fusion power plant, irradiation is not the only factor affecting reflectivity. Mirror test in JET [44] has shown that reflectivity is strongly decreased (by 50-85%) due to Be, C, N, O and W deposition. Also, loading of mirror surface with hydrogen isotopes would influence the reflectivity. In that respect, reflectivity measurements on samples that contain deuterium (before TDS) are desirable. In the case that maintenance of the mirrors is required due to degradation of the optical properties, it may be desirable to reduce the tritium contamination prior to mirror cleaning. These results indicate that even after irradiation, the majority of tritium can be thermally desorbed without significant impact on the optical properties.

3.2. Modelling

During the Frenkel pairs accumulation method simulations, it is necessary to measure damage such as vacancies and self-interstitials that is accumulated in the system. Number of vacancies in the system was calculated using two methods. First, Wigner-Seitz defect analysis as implemented in OVITO software [45], was used. This is a global method in which it is presumed that single crystal remains intact during the simulation. However, it is quite possible that smaller crystallites will arise as a result of rotation and splitting the initial single crystal. To check for this possibility, a local criterion was used to calculate number of single vacancies. After energy minimization from a given configuration, for each Mo atom, number of its nearest neighbours was calculated. If this number was equal to 7, one less than in a perfect bcc crystal, the position of the missing atom was considered to be a vacancy. To ensure that this is a single vacancy, it was checked that there are eight nearest neighbour Mo atoms that locate the vacancy

in the same position (maximal distance between vacancy locations of 1 Å was allowed). This method misses vacancy clusters and thus underestimates total number compared to the Wigner-Seitz analysis; however, it is stable with respect to splitting initial single crystal into smaller crystallites. Our results showed that for T = 300 K and T = 600 K, Wigner-Seitz analysis consistently gave number of vacancies 20% to 40% higher than the local criterion. However, for the case of T = 900 K, number of vacancies as calculated by Wigner-Seitz analysis fluctuated hugely, up to 10 times between subsequent configurations, while the local criterion gave similar results. This suggests that at this high temperature, the single crystal indeed splits during the simulations, and the Wigner-Seitz analysis gives incorrect results. Consequently, only the local criterion was used.

Total amount of single vacancies in the system as function of canonical dpa calculated using local criterion is shown in Figure 6. For T = 300 K, it saturates at concentration of around 1.5 at. % under canonical damage of around 0.2 dpa. For higher irradiation temperature of 600 K, vacancy content hardly changes, but at 900 K, decrease in number of single vacancies was found, with saturation at around 1 at. %. Similarly to the case of 300 K, saturation at higher temperatures is achieved at around canonical damage of 0.2 dpa. It is clear that there is qualitative agreement between number of vacancies obtained using modelling and the experimental results on the total deuterium inventory shown in Figure 4.

4. Discussion

In order to understand the origin of features in TDS spectra of unirradiated and irradiated molybdenum samples, it is instructive to compare molybdenum results with our results on tungsten ([43], Figure 6 therein). Similar to molybdenum, in the case of tungsten, several characteristic temperature regions were identified, but in W they are more clearly separated. Low-temperature (550-600 K) tungsten peak is present in the spectra of all samples, while in the molybdenum, the 400-450 K peak can be clearly seen only in unirradiated sample and becomes a shoulder in irradiated samples. As in the case of tungsten, this low-temperature feature can be related to both intrinsic defects, such as grain boundaries or surface adsorption sites [46], and irradiation-induced defects, including vacancies with multiple occupation, as it was shown for tungsten that as the occupancy of traps increases, the binding energy of hydrogen isotopes decreases [47,48]. Further studies, including *ab initio* modelling, are needed

to identify possible single origin of that peak, or to confirm that it stems from both intrinsic and irradiation-related defects.

The main peak in irradiated Mo samples is at around 550 K, close to operating temperature of optical diagnostics mirrors [13,14], while in W it is centred around 700-750 K. This peak is present even in a sample irradiated to lowest damage of 0.01 dpa and is probably seen as a shoulder in unirradiated sample. Similarly to the case of tungsten, this peak is attributed to deuterium release from single vacancies, most of which are created by irradiation. Next, a shoulder-like feature can be seen just above 600 K in sample Mo41 irradiated up to 1 dpa. The 600 K feature is not seen in sample Mo42 that was measured next day after exposure to deuterium, because it is completely masked by the main peak. It is only revealed in sample Mo41 measured after 1 month delay, after part of deuterium has been released from vacancies. This confirms it is a deep trap feature that remains stable after more weakly bound single vacancy deuterium desorbs during the hold time of one month. Finally, a small broad peak was detected at around 1100 K in all the irradiated samples, with its height increasing with the increase of irradiation dose. The absence of this feature in the unirradiated sample indicates that it is related to deuterium trapping in the defects associated with the displacement damage. Similar high-temperature release peak in tungsten is attributed to the release of deuterium from the gas-filled under-surface voids or vacancy clusters [49,50], and we believe the 1100 K peak in Mo has similar origin.

Our attribution of some of TDS features is in disagreement with that in [20]. In our opinion, the main TDS peak around 550 K is related to single vacancies and other damage created by irradiation, and not to retention of deuterium in natural traps, as suggested in [20]. Our suggestion is confirmed by sharp rise of that peak after irradiation, and also by saturation of its height between the canonical damage of 0.1 dpa and 1 dpa. This peak is responsible for most of deuterium inventory at damage above 0.01 dpa, and its origin is further confirmed by our modelling results. It was found that the increase and following saturation of vacancy concentration found in simulations using Frenkel pair accumulation method follows increase and following saturation of deuterium content and the height of 550 K peak as found by TDS experiment. Another important result of modelling studies is the similarity of vacancy concentrations at saturation for different simulation temperatures. For temperatures of 300 K and 600 K, number of single vacancies found is similar, while at T = 900 K, a decrease in number of single vacancies by 20-30%, down to 1 at. %, was found. This suggests that

experimental irradiations performed at room temperature create damage and, consequently, hydrogen intake similar to those obtained at the temperature of fusion power plant.

Our results on reflectivity indicate that the optical properties of molybdenum are hardly affected by self-irradiation with damage up to 1 dpa. This is in agreement with recent study [22], where even 30 dpa dose of low-energy (30 keV) Mo self-irradiation resulted in a slight decrease of the total reflectivity. In the following work [23], it was found that the implantation of other 30 keV heavy ions, ^{93}Zr and ^{90}Nb, up to the dose corresponding to the damage of 10 dpa does not change reflectivity in the near ultraviolet and visible range. Our results show that high-energy Mo ions also do not lead to a noticeable degradation of reflectivity. In the subsequent studies, it is important to measure reflective properties of Mo on both irradiated and exposed to deuterium samples, closer to realistic conditions. Also, studies of repeated exposure to hydrogen isotopes followed by thermal desorption will improve the understanding of the longevity of Mo optical components in the harsh environment of fusion reactors.

5. Conclusions

The first study of deuterium retention and reflectivity for molybdenum self-irradiated up to a high dose of 1 dpa by high energy (1 MeV) ions has been performed. Our results show several features of the TDS spectrum, with most prominent of them, large peak at around 550 K, increasing with irradiation damage. Experimental results together with Frenkel pair accumulation modelling indicate this peak as resulting from deuterium trapped in single vacancies and other damage created by irradiation. The increase and following saturation of vacancy concentration found in simulations using Frenkel pair accumulation method, Figure 6, follows increase and saturation of deuterium content above canonical damage of 0.1 dpa as found in experiment, Figure 4. Modelling further indicates weak dependence of vacancies concentration on the irradiation temperature. Another important result of the modelling study that should be pursued further is the difference between global (Wigner-Seitz) and local criteria in calculating the number of vacancies, especially at high temperature. Reflectivity of molybdenum is hardly affected by irradiation with damage up to 1 dpa, being the same within 1.5%, which is within measurement uncertainty. This confirms suitability of molybdenum for being used as a mirror in optical diagnostics systems of fusion power plant. Still, further studies on samples exposed to deuterium are needed.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Sample	Self-ion irradiation fluence (1 MeV Mo^{+} ions)	Approximate self-ion irradiation dose (dpa)	Deuterium implanted?	Characterization
Mo2	1.05×10^{14}	1	No	Reflectivity
Mo3	1.05×10^{12}	0.01	No	Reflectivity
Mo4	1.05×10^{13}	0.1	Yes	TDS
Mo6	1.05×10^{13}	0.1	No	Reflectivity
Mo7	0	0	Yes	TDS
Mo18	1.05×10^{12}	0.01	Yes	TDS
Mo41	1.05×10^{14}	1	Yes	TDS
Mo42	1.05×10^{14}	1	Yes	TDS

Table 1. List of the samples used in the current study.

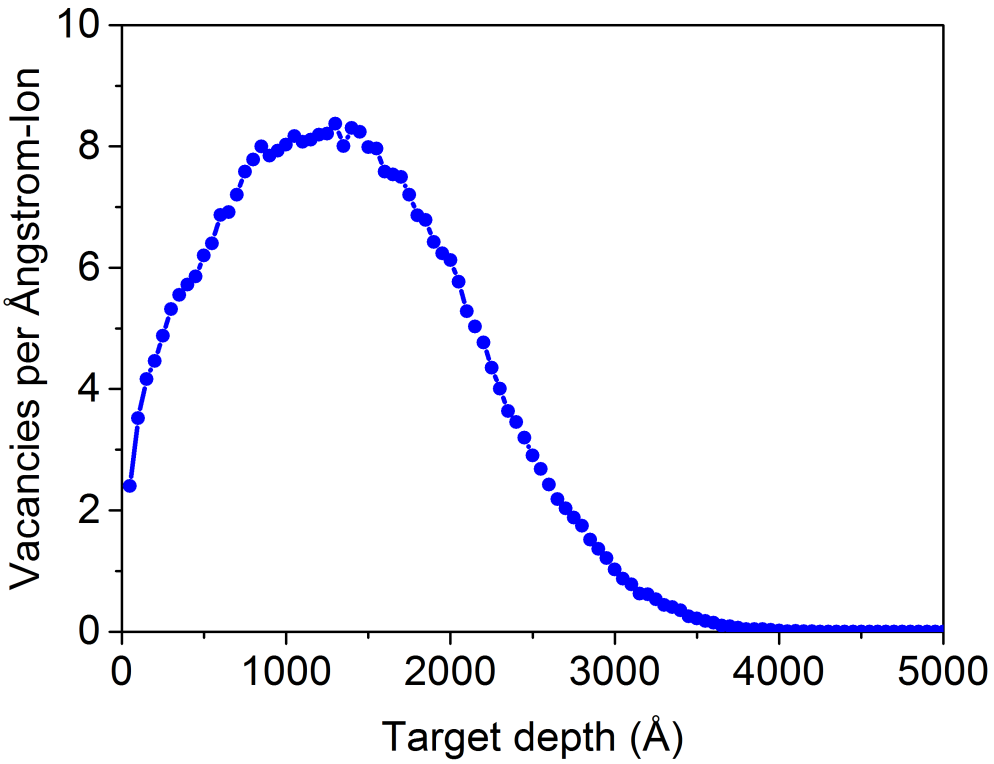

Figure 1. Number of vacancies created per incoming ion in 1 Å thick layer as function of depth as obtained using SRIM software for 1 MeV incoming Mo ions.

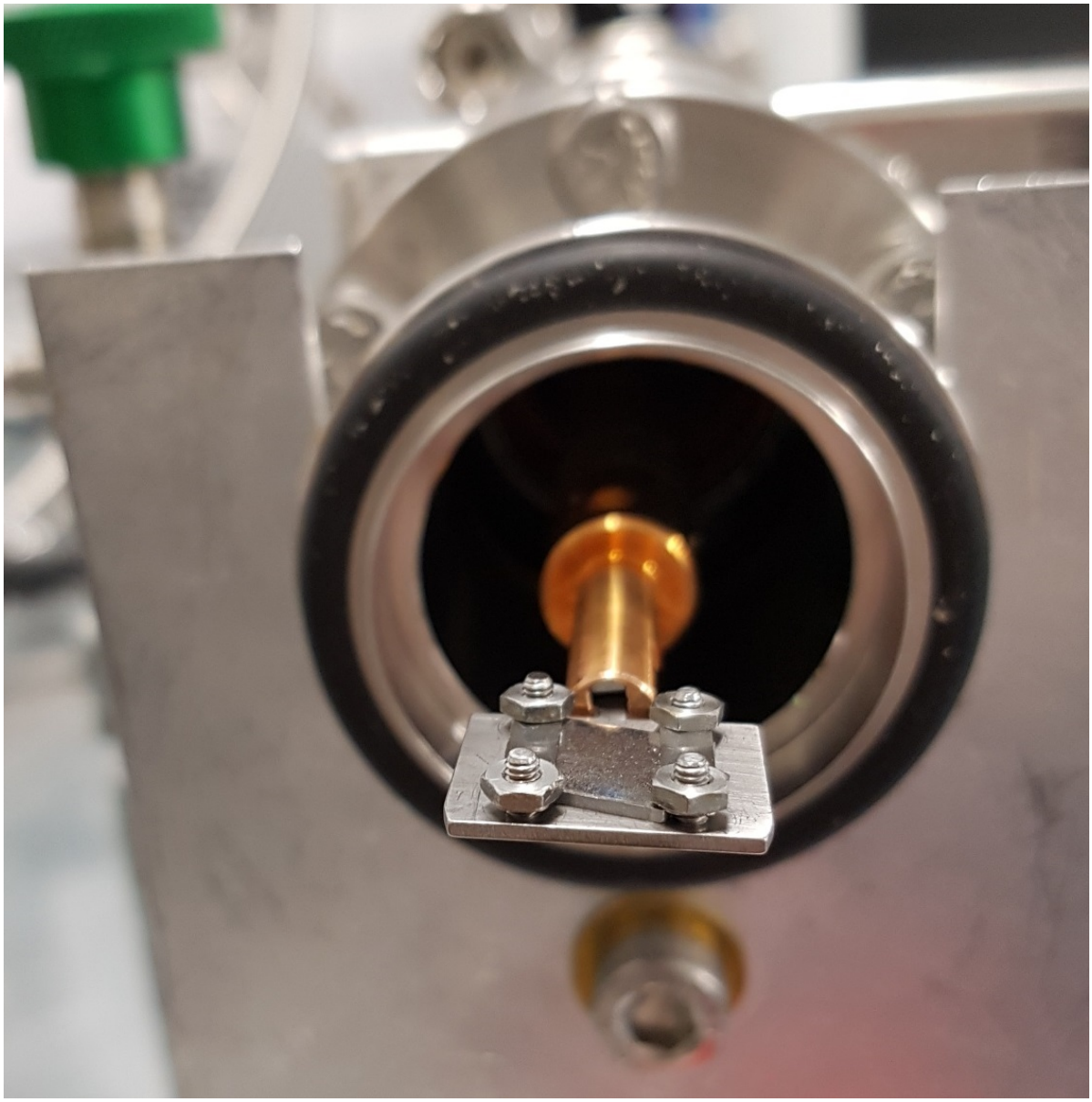

Figure 2. Molybdenum sample mounted to the sample holder.

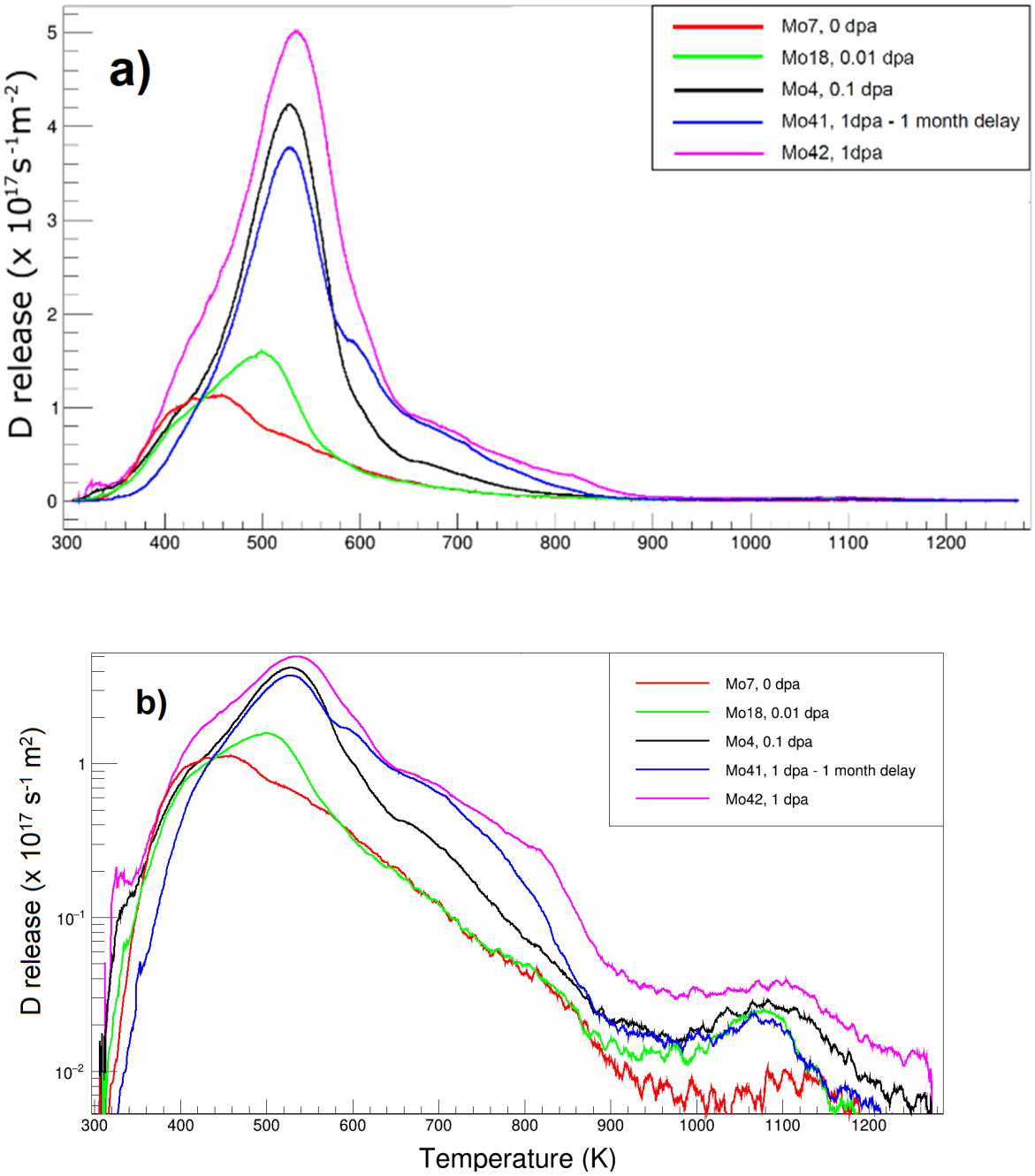

Figure 3. TDS spectra of deuterium in Mo samples with damage levels between 0 and 1 dpa. For samples Mo18, Mo4, and Mo42, spectra were taken 1 day after exposure to D plasma; for the sample Mo41, spectrum was taken 1 month after exposure. Linear plot (a); logarithmic plot (b).

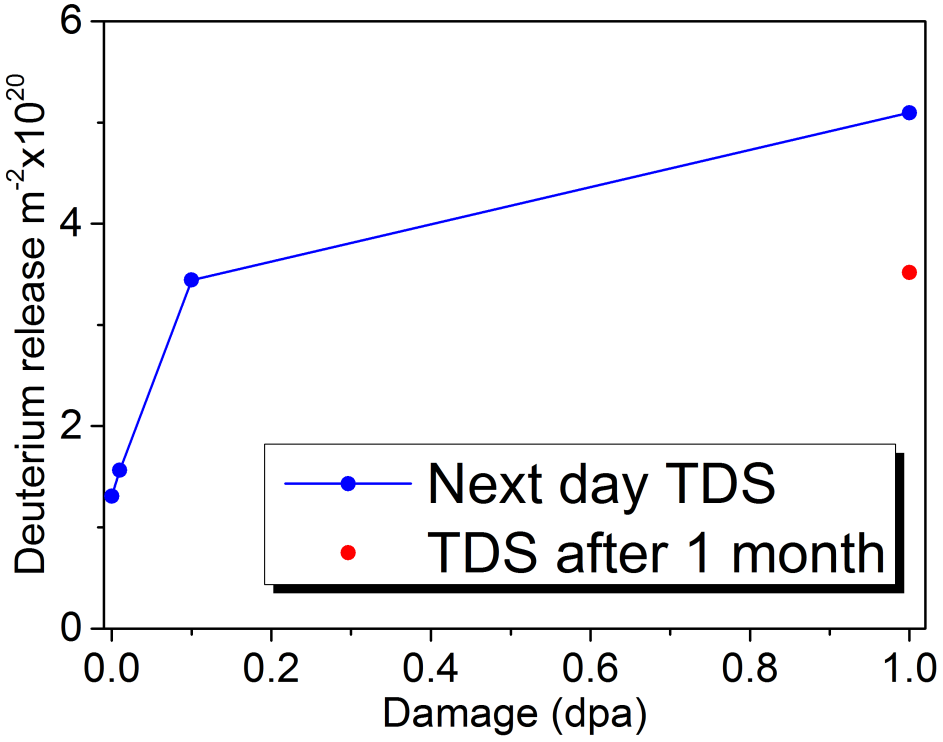

Figure 4. Overall deuterium inventory as function of canonical damage. For 1 dpa samples, results are shown for TDS performed next day (Mo42, blue point) and one month (Mo41, red point) after exposure.

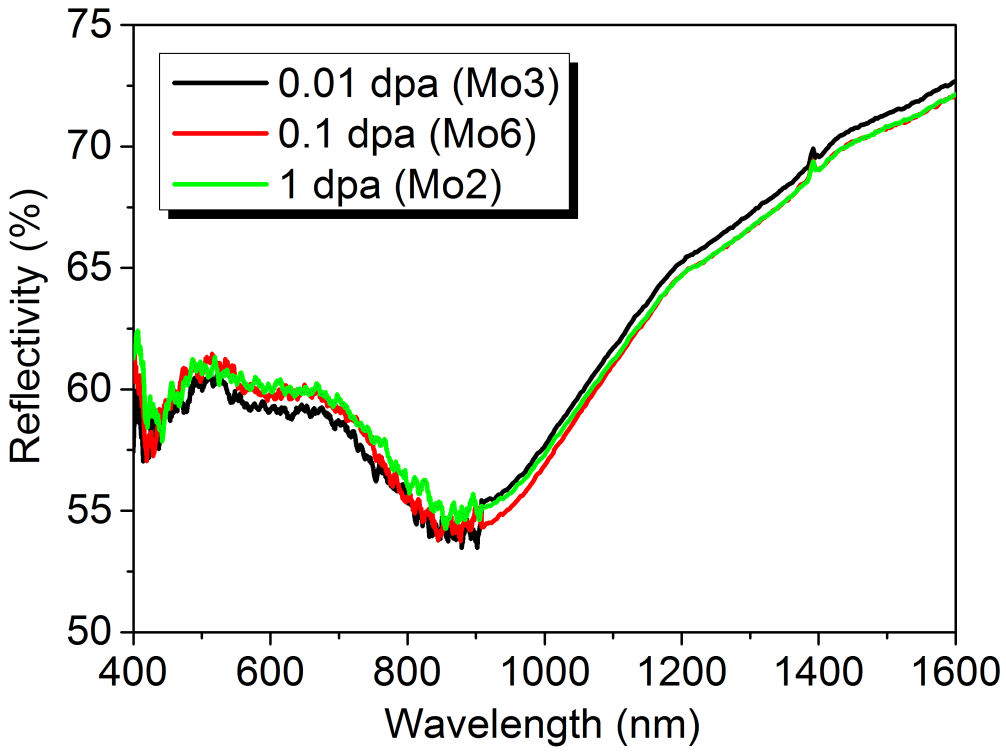

Figure 5. Total Mo reflectivity as a function of wavelength for samples irradiated to 0.01 dpa (Mo3), 0.1 dpa (Mo6), and 1 dpa (Mo2).

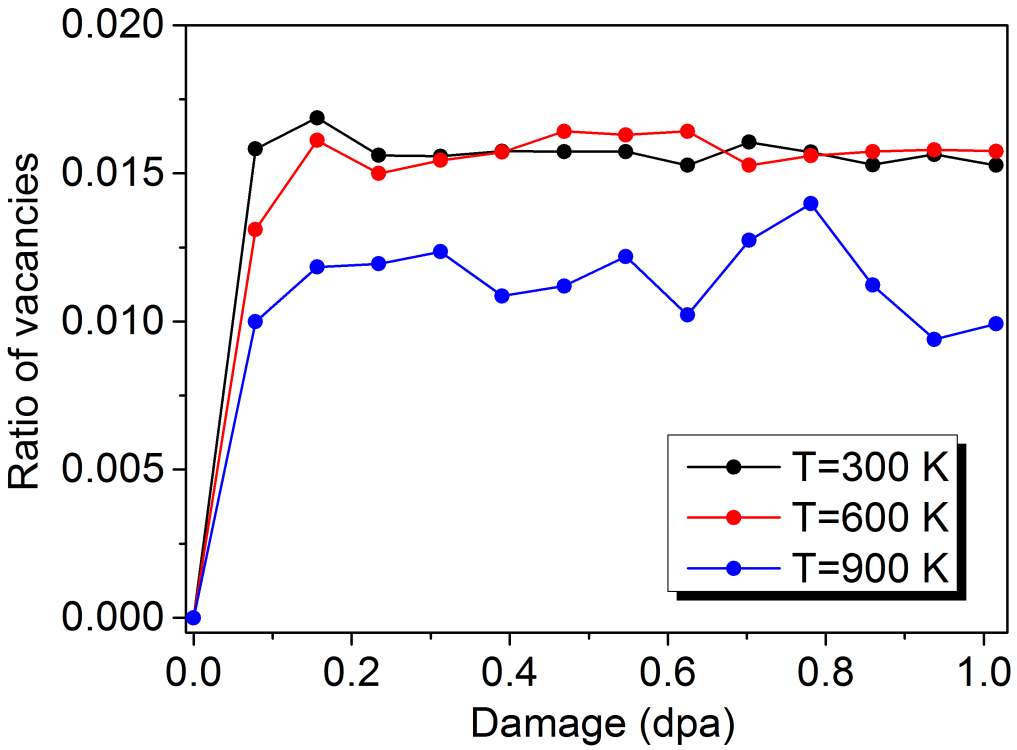

Figure 6. Ratio of single vacancies created in molybdenum as function of canonical damage introduced by Frenkel pair accumulation method at different temperatures.