



# Expanding the capability of reaction-diffusion codes using pseudo traps and temperature partitioning: Applied to hydrogen uptake and release from tungsten



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## ABSTRACT

Simulating the implantation and thermal desorption evolution in a reaction-diffusion model requires solving a set of coupled differential equations that describe the trapping and release of atomic species in Plasma Facing Materials (PFMs). These fundamental equations are well outlined by the Tritium Migration Analysis Program (TMAP) which can model systems with no more than three active traps per atomic species. To overcome this limitation, we have developed a Pseudo Trap and Temperature Partition (PTTP) scheme allowing us to lump multiple inactive traps into one pseudo trap, simplifying the system of equations to be solved. For all temperatures, we show the trapping of atoms from solute is exactly accounted for when using a pseudo trap. However, a single effective pseudo trap energy can not well replicate the release from multiple traps, each with its own detrapping energy. However, atoms held in a high energy trap will remain trapped at relatively low temperatures, and thus there is a temperature range in which release from high energy traps is effectively inactive. By partitioning the temperature range into segments, a pseudo trap can be defined for each segment to account for multiple high energy traps that are actively trapping but are effectively not releasing atoms. With increasing temperature, as in controlled thermal desorption, the lowest energy trap is nearly emptied and can be removed from the set of coupled equations, while the next higher energy trap becomes an actively releasing trap. Each segment is thus calculated sequentially, with the last time step of a given segment solution being used as an initial input for the next segment as only the pseudo and actively releasing traps are modeled. This PTTP scheme is then applied to experimental thermal desorption data for tungsten (W) samples damaged with heavy ions, which display six distinct release peaks during thermal desorption. Without modifying the TMAP7 source code the PTTP scheme is shown to successfully model the D retention in all six traps. We demonstrate the full reconstruction from the plasma implantation phase through the controlled thermal desorption phase with detrapping energies near 0.9, 1.1, 1.4, 1.7, 1.9 and 2.1 eV for a W sample damaged at room temperature.

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## 1. Introduction

The modeling of tritium fuel trapping and retention within neutron damaged W is of primary concern to next step fusion devices. In addition to the degradation of material properties, the accumulation of tritium has safety requirements regulated by the Nuclear Regulatory Commission [1]. Aside from transmutation and

radioactivity, many of the fundamental aspects of neutron damage and tritium retention can safely be studied with the use of heavy ions and deuterium (D), respectively.

The primary experimental techniques for studying hydrogenic retention in W are Nuclear Reaction Analysis (NRA) and Thermal Desorption Spectroscopy (TDS). NRA utilizes a <sup>3</sup>He ion beam to probe the D concentration up to several microns in depth. This technique does not differentiate as to which type of trap holds the D, nor if it is in solution between lattice sites, but can infer the spatial distribution of D contained within the damaged materials.

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With TDS, the sample temperature is linearly increased and the surface flux of desorbed D is measured as a function of temperature. The flux of D from the sample is complicated by the multi-step migration process of diffusion, trapping, release, and eventual surface recombination to escape the sample. By modeling these coupled processes, TDS can reveal the energy required to escape a given trap. The release behaves as an Arrhenius process, in that an atom is trapped within an energy barrier and may escape once the atom acquires enough kinetic energy via random collisions.

Previous experiments studying the release of D from W through TDS have observed a range of release peaks at different temperatures, leading to a variety of inferred detrapping energies ranging from 0.65 to 2.4 eV [2–7]. Release peaks may shift in temperature due to various experimental effects. In the case of heavy ion damaged samples, the most significant factor that affects the release peaks is the damage depth profile. Samples with D filling traps formed by damage cascades deeper within the material will have further to migrate before reaching the surface, and thus have a higher probability of retrapping prior to reaching the surface, which leads to a broadening of the release peak and a shift towards higher temperature. Analysis of the release peaks is further obfuscated by the overlapping and coupling of traps due to a range of detrapping energies. In addition, traps with low detrapping energies may be missed entirely when sample temperature during the atomic implantation phase approaches or exceeds its low temperature release peak, preventing that trap from being populated and subsequently inferred through NRA or TDS measurements.

Though no ion source will produce the same damage as 14 MeV fusion neutrons, many of the resultant defects' fundamental properties can be explored. We do note that experiments utilizing ion damage may have experimental data that in turn produces more reliable inferred detrapping energies. Samples with uniform trap concentrations, such as undamaged or neutron damaged samples, may never saturate the filled trap concentration causing atoms escaping low energy traps to diffuse and further populate high energy traps deeper into the material. This can result in the filling of traps that are located beyond 10  $\mu\text{m}$  depth. The subsequent TDS of such traps results in significant broadening of the release peaks, causing adjacent peaks to overlap and further obscuring the inferred detrapping energies. Unlike an undamaged or neutron damaged sample, the damage profile from heavy ions has a distinct depth and shape localized to the near surface region that can be modeled with the Stopping Range of Ions in Material (SRIM) [9]. Using this ion-induced damage spatial profile as a constraint, the resultant release peaks seen in experimental TDS data have a specific origin, increasing the confidence in the inferred detrapping energies. Note that the dpa profile predicted by SRIM does not take temperature into account [10]. The annealing of defects during or post damage will alter the shape of the profiles for surviving defects.

In order to infer the detrapping energies from TDS release peaks, a reaction-diffusion model must be used to simulate the experimental conditions. The Tritium Migration Analysis Program (TMAP) is a well validated and verified code used extensively within both the fission and fusion communities to simulate hydrogenic retention measurements [11–13]. The current version of TMAP7 can model up to three coupled traps simultaneously and was used to model the D implantation and thermal desorption phases of a recent experiment [14]. In our present work, we find that three traps cannot reasonably model the experimental data. To model a larger number of traps concurrently within the TMAP7 framework, we introduce a new PTPP scheme and show that it can effectively model the trapping and release of D from damaged W that exhibits trapping and release in six distinct traps.

## 2. TMAP7 simulation

As described in detail in Ref. [14], W samples were simultaneously damaged and annealed prior to D implantation in the PISCES-E RF plasma device. The simulation of D retention in W can be separated into three phases: the sample preparation, D implantation, and thermal desorption of D. Phase 0, sample preparation, produces the initial concentration of various defects that act as traps. Phase I, D implantation, entails the diffusion of D within the W lattice and the gradual filling of traps encountered by the diffusion front. Phase II, thermal desorption, is defined by the release of D from filled traps by controlled heating of the W sample. Table 1 below provides a summary of the relevant experimental parameters utilized in this simulation. In what follows, the sample damaged at room temperature is modeled.

Simulating the implantation phase, values for mean implantation depth ( $\sim 4$  nm) and surface ion reflection coefficient ( $\sim 0.65$ ) were taken from Eckstein [15]. To achieve consistency between modeled depth profile, thermal desorption, and experiment, either recombination, reflection, or re-emission must be increased for high incident ion flux during the implantation phase. The peak solute D concentration in the implantation zone is limited by one of these processes. This peak concentration also determines the D gradient that in turn drives the overall D diffusing into the bulk where it can be retained. Here the recombination coefficient could be taken as instantaneous to shift the release rate limiting process from surface release to diffusion. Instead, in order to retain the physics of recombination during the thermal desorption phase, we chose to increase the surface ion reflection coefficient ( $R$ ) above the quoted Eckstein value. The incident ion flux ratio,  $\Gamma_{in}/\Gamma_{ion}$ , that penetrates the surface and is then implanted, was taken to be  $8 \times 10^{-4}$ , where  $\Gamma_{in}/\Gamma_{ion} = 1 - R$ . This degree of reduction is consistent with what was required to match results in other relatively high ion flux experiments [16]. Note that a similar implantation profile can be achieved using Eckstein's reflection coefficient when recombination is neglected and instantaneous surface release is modeled. The mechanism that reduces the D retained during implantation needs further experimental investigation. This is currently an unresolved issue that highlights the difficulty in the application of reaction diffusion physics to the uptake of hydrogenic isotopes in tungsten.

The D filled trap sites shown in the NRA experimental data (thick black) in Fig. 1 occupy three different spatial zones: the near surface implantation zone ( $\sim 70$  nm), the heavy ion damage zone ( $\sim 1$   $\mu\text{m}$ ), and the intrinsic defects throughout the rest of the sample. The W samples were initially annealed below the recrystallization temperature, which leaves behind a presumably uniform distribution of residual intrinsic defects. A uniform concentration of intrinsic traps was therefore assumed throughout the 1.5 mm thick sample. The spatial profile of D detected by NRA largely coincides with the spatial location of heavy ion damage predicted by SRIM [8]. As a result, in this work the concentration of Cu ion induced defects shown in Fig. 1 is assumed to have the SRIM spatial profile (red). Within 70 nm of the surface region, the NRA measurements of D retention shows defects were created and populated by D implantation, possibly due to lattice stresses induced by the incident plasma ion flux [6,17]. Shown on the log-log plot, the implantation zone is a small contribution to the total D retention and, therefore, simply modeled as a step function up to 70 nm. Since NRA measures the sum of all D filled traps, the detrapping energy of each trap cannot be determined without simulating the thermal desorption phase. As such, the concentration of each trap within each of these three zones is a free parameter, constrained by both the sum of filled traps after implantation (i.e. the spatial D profile from NRA) and the surface flux profile from TDS.

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