SIMULATION OF FUEL INVENTORY IN DAMAGED TUNGSTEN UNDER SIMULTANEOUS HYDROGEN AND DEUTERIUM: SYNERGISTICAL EFFECT OF DEFECT ANNEALING AND ISOTOPE EXCHANGE

Zhenhou Wang[1], Chaofeng Sang[1]*, Mengtao Li[1], Haiong Du[1], Dezhen.Wang[1]

[1] Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), School of Physics, Dalian University of Technology, Dalian 116024, China
[2] Southwestern Institute of Physics, Sichuan, Chengdu 610041, China

Email: sang@dlut.edu.cn

The management of tritium (T) inventory in plasma-facing materials (PFMs) for future fusion reactors is a critical concern due to radiological safety risks associated with tritium retention [1]. Consequently, stringent control of T accumulation in PFMs is imperative. Tungsten (W) has emerged as the primary candidate for PFMs owing to its favourable properties, including low intrinsic T retention. However, during tokamak operation, PFMs are subjected to simultaneous bombardment by hydrogen isotope (HI) ions (D, T) and high-energy neutrons, leading to the formation of lattice defects that exacerbate T retention. Notably, 14 MeV neutron irradiation generates dense populations of defects with high trapping energies (e.g., vacancy clusters, voids), which dominate T inventory build-up in DT fusion scenarios[2]. Extensive research has focused on predicting HI retention in neutron-damaged PFMs. A significant limitation persists: direct experimental studies of neutron-induced damage remain scarce, necessitating the use of ion irradiation as a proxy[3,4]. Recent experimental and computational advances have elucidated key mechanisms, demonstrating that trapping and de-trapping kinetics at radiation-induced defects govern fuel retention[5][6]. Nevertheless, prevailing studies exhibit two critical shortcomings. On one hand, most retention data derive from single-species HI irradiation, neglecting synergistic effects of mixed H/D/T fluxes characteristic of reactor plasmas. The isotopic effects on HI retention under multi-species HI irradiation is interesting, e.g., isotope exchange effect. On the other hand, defect evolution dynamics (e.g., recombination, clustering) under prolonged irradiation are rarely incorporated, despite their profound influence on trap site populations. The evolution of defects in PFMs is a stochastic, non-linear process governed by competing mechanisms such as defect annealing and hydrogen isotope (HI) trapping-de-trapping kinetics. Experimental study of this dynamic evolution remains prohibitively challenging, consequently, advanced multiscale numerical modelling becomes indispensable to unravel defect-HI synergies and predict T inventory in PFMs under reactor-relevant conditions.

In our previous work [7], we developed a Hydrogen Isotope Inventory Process Code (HIIPC) to assess fuel retention in self-ion damaged W under sequential D and H irradiation, and found that the trapped D is reduced during H irradiation due to the occurrence of the isotope exchange (H → D). However, our preliminary results demonstrated that the reduce D retention by isotopic exchange is limited due to static defect assumption and oversimplified exchange. To address these gaps, our recent work [8] established a dynamic defect evolution model that quantifies vacancy/interstitial-type defect populations under simultaneous W-ion bombardment and thermal annealing, providing time-resolved trap site densities for HI retention.

In the present work, building upon our previous works[7–9], we further upgraded the HIIPC that incorporates multi-species HI bombardment and defect dynamics coupling to simulate H and D retention in radiation-damaged W under concurrent H/D irradiation. The primary objective is to elucidate the synergistic interplay between defect annealing kinetics and isotopic exchange mechanisms in governing HI retention. First, the retained concentrations of H and D at static damaged trap concentration are simulated under simultaneous irradiation of H and D flux at certain temperature. A strong competition between H and D for trap site is observed, indicating that D exhibits preferential trapping at vacancy-type defects due to its higher trapping energy than H. Next, the D retention under simultaneous H/D fluxes and evolving defect populations is evaluated. A synergistic role of vacancy-type traps annealing and H/D exchange in reducing D retention is revealed, and their contributions to total D amount is quantified. Also, the influencing factors of the reduced retention D are discussed at a wider parametric range of temperatures and H/D fluxes. The simulation results show that the H/D exchange shows great contribution to the reduced D retention at low temperature, while, as the increasing of temperature, the defect annealing and thermal de-trapping show an increasing important contribution, thus facilitating to the D inventory control. It is also found that raising the ratio of H/D flux can remarkably decrease the trapped D concentration due to the isotope exchange (H→D). In summary, this model firstly integrates defect dynamics with isotopic exchange, offering predictive insights into HI inventory control in fusion reactor PFMs.

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