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

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ABSTRACT

- A strong competition between H and D for trapping sites was observed, indicating that D is preferentially trapped at vacancy-type defects than that of H.
- The synergistic effect of vacancy-type trap annealing and isotope exchange in reducing D retention.
- The simulation results demonstrate that H/D exchange contributes to the reduction of D retention at low temperatures. As the temperature increases, defect annealing and thermal detrapping play increasingly important roles, which is beneficial to lower D inventory.
- It was found that increasing the H/D flux ratio decreases the trapped D concentration due to competitive exchange.

BACKGROUND

- The trapping and de-trapping kinetics at radiation induced defects govern fuel retention. The isotopic effects on HI retention under multi-species HI irradiation is interesting, e.g., isotope exchange effect.
- Most retention data derive from single-species HI irradiation, neglecting synergistic effects of mixed H/D/T fluxes characteristic of reactor plasmas.
- The defect evolution dynamics (e.g., recombination, clustering) under prolonged irradiation are rarely incorporated in multiple species irradiation, despite their profound influence on trap site populations.
- To systematically simulate multiple HI retention behavior in W, we simulated the D retention in W under the irradiation with W ions, H and D plasmas, with particular emphasis on the coupling between defect evolution and isotope exchange mechanisms.

SIMULATION MODEL

- The VITDE-HIIPC model has been developed to describes the co-evolution of three key field quantities under multi-species particle bombardment : the concentrations of irradiation-induced interstitial-type defect clusters (I_n), vacancy-type defect clusters (V_n), and HI (H and D).
- The defects interact with implanted H/D through a series of key processes—including diffusion, reaction, clustering, dissociation, trapping, and de-trapping—whose rates are governed by physical parameters.

The equations of VITDE-HIIPC model can be expressed as followings:

$$\frac{\partial C_{I_n}(z,t)}{\partial t} = G_{I_n} + D_{I_n}(T)\frac{\partial^2 C_{I_n}}{\partial z^2} - \frac{\partial C^{clust}_{I_n-I_m}}{\partial t} - \frac{\partial C^{recom}_{V_n-I_m}}{\partial t} - \frac{\partial C^{D}_{I_n}}{\partial t} - \sum_{i=1}^{M}\frac{\partial C^{I_n}_{sink,i}}{\partial t}$$

$$\frac{\partial C_{V_n}(z,t)}{\partial t} = G_{V_n} + D_{V_n}(T)\frac{\partial^2 C_{V_n}}{\partial z^2} - \frac{\partial C^{clust}_{V_n-V_m}}{\partial t} - \frac{\partial C^{recom}_{V_n-I_m}}{\partial t} - \frac{\partial C^{D}_{V_n}}{\partial t} - \frac{\partial C^{H}_{V_n}}{\partial t} - \sum_{i=1}^{M}\frac{\partial C^{V_n}_{sink,i}}{\partial t}$$

$$\frac{\partial C^{D}_{s}(z,t)}{\partial t} = G_D + D_D(T)\frac{\partial^2 C^{D}_{s}}{\partial z^2} - \sum_{i=1}^{M}\frac{\partial C^{D}_{sink,i}}{\partial t} - \sum_{n=1}^{N}\frac{\partial C^{D}_{V_n}}{\partial t}$$

$$\frac{\partial C^{H}_{s}(z,t)}{\partial t} = G_H + D_H(T)\frac{\partial^2 C^{H}_{s}}{\partial z^2} - \sum_{i=1}^{M}\frac{\partial C^{H}_{sink,i}}{\partial t} - \sum_{n=1}^{N}\frac{\partial C^{H}_{V_n}}{\partial t}$$

$$\frac{\partial C^{D}_{V_n}}{\partial t} = \omega^{+}_{D,V_n} C^{D}_{s} C_{V_n} - \omega^{-}_{D+V_n} C^{D}_{V_n} exp\left(-\frac{E^{dt}_{V_n-D}}{k_b T}\right) - v_0 e^{-\frac{E_{swap}}{k_b T}}\left(\frac{C^{H}_{s}C^{D}_{t} - C^{D}_{s}C^{H}_{t}}{N_T}\right)$$

$$\frac{\partial C^{H}_{V_n}}{\partial t} = \omega^{+}_{D,V_n} C^{H}_{s} C_{V_n} - \omega^{-}_{D+V_n} C^{H}_{V_n} exp\left(-\frac{E^{dt}_{V_n-H}}{k_b T}\right) - v_0 e^{-\frac{E_{swap}}{k_b T}}\left(\frac{C^{D}_{s}C^{H}_{t} - C^{H}_{s}C^{D}_{t}}{N_T}\right)$$

OUTCOME

The effect of damage level (dpa) on H and D retention and trap production

- Under simultaneous irradiation, a strong competition between H and D for trapping sites was observed, indicating that D is preferentially trapped at vacancy-type defects than that of H.
- As the dpa increases, maximum values of trapped H and D all rise, while their penetration depths decrease, and the trapped H, D enhance traps.

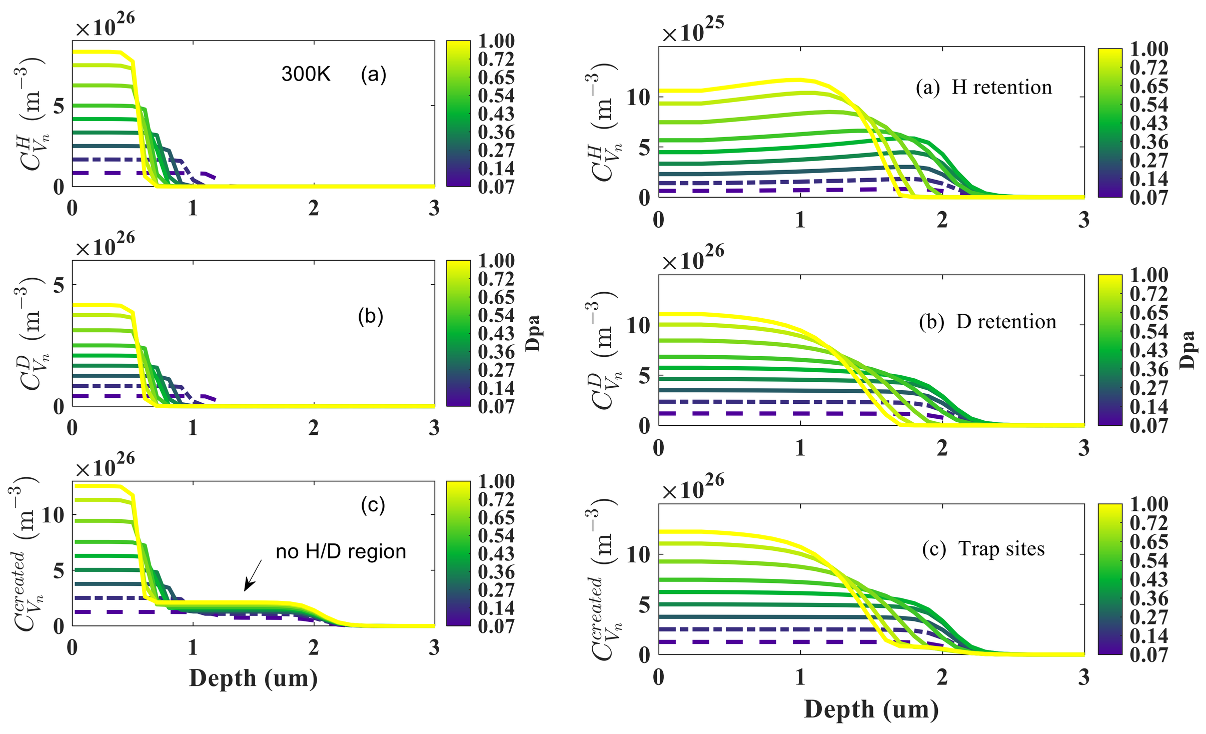
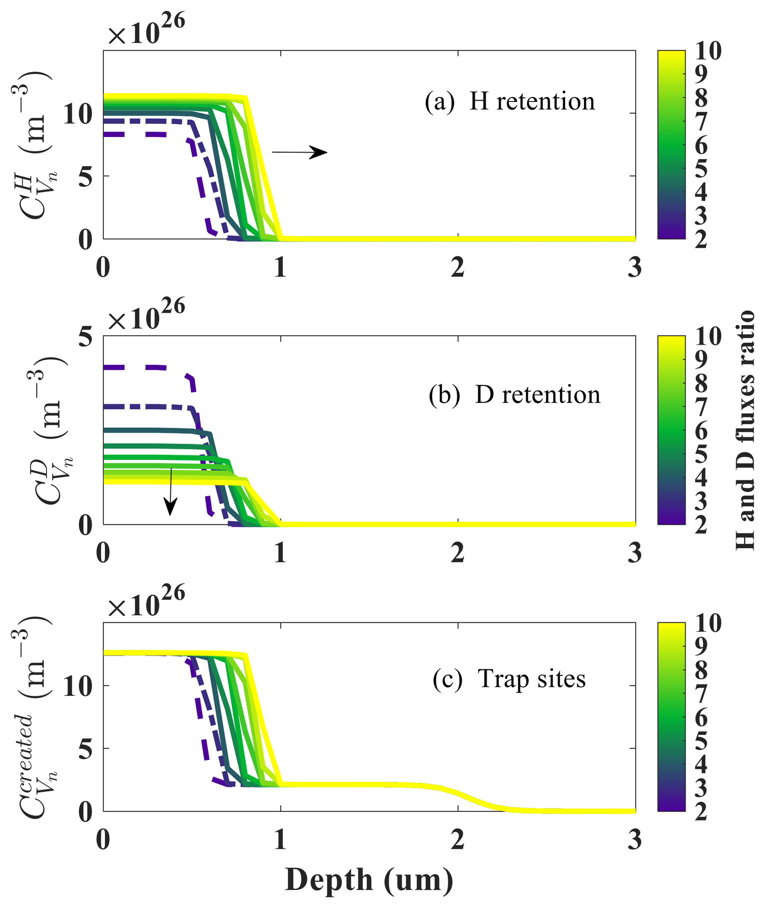


Fig. 1. Variations of H, D and induced traps concentrations as dpa raises in W after simultaneous at 300K and 600K. The irradiation time 1h and the W-ion damage rate of $2{\times}10^{-4}$dpa/s.

The effect of H and D flux ratio on H and D retention and distributions

- Under simultaneous irradiation, as the H/D flux ratio increases, the maximum concentration of trapped H rises , while that of trapped D declines.
- Increasing H/D flux ratio shows a strong H exchange for D, and following the cessation of the D flux, trapped D is further reduced as H irradiation fluence increases.



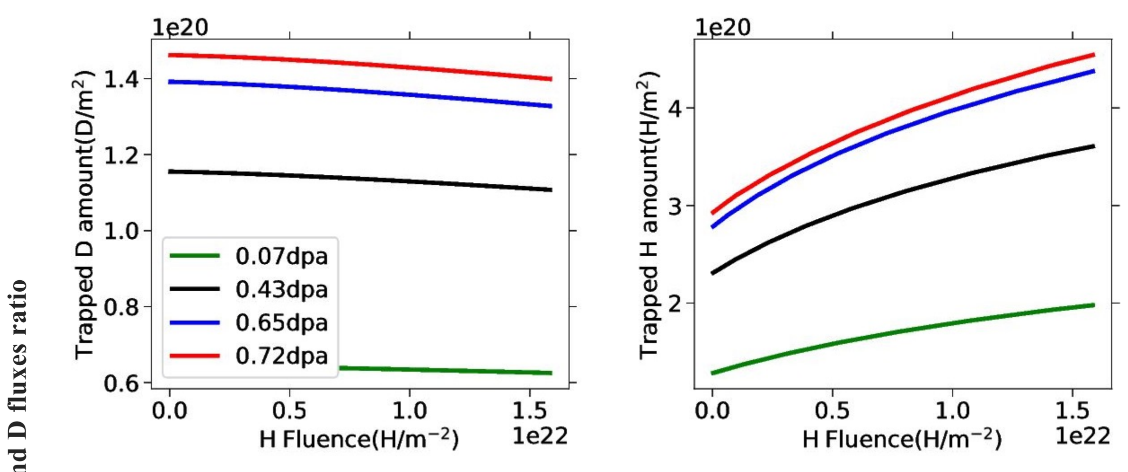


Fig. 2. Variations of H, D and induced traps concentrations with H and D flux ratio and further isotope exchange in W after simultaneous high energy W ions and low energy HI particles at 300K.

CONCLUSION

- The simulation confirms that the retention of H/D and their interactions with irradiation-induced defects depends on defect annealing and isotope exchange.
- The retention densities of both H and D rises with increasing radiation damage, and the higher damage rates increase defect generation and enhance H and D trapping in damaged W.
- The trapped H/D density shows a strong dependence on material temperature and the H/D flux ratio. At lower temperatures, H retention exceeds that of D, whereas this trend reverses at elevated temperatures. Increasing the H/D flux ratio at low temperatures effectively reduces trapped D.

ACKNOWLEDGEMENTS / REFERENCES

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