Molecular dynamics simulation study of the deuterium retention in tungsten exposed to low-energy, high fluxes of pure D and He-D mixture

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Molecular dynamics simulation has been performed to study deuterium behavior in tungsten exposed to pure and helium-deuterium mixture bombardments at surface temperature 300-2000 K. Our findings show that deuterium retention in W decreased with increasing temperature, and the amount of D retained in W decreased with increasing fluence of pure D bombardment. In contrast, it was found that the amount D retained in W decreased much more significantly with D-He mixture (He, 10\textendash{}20 \%) bombardment at a temperature at 500 K and above, while at room temperature the D retention was enhanced instead, which indicated there existed a critical temperature between 300 and 500 K for the transition. The incident flux of D-He mixture bombardment affected the permeation of D in W by limiting D diffusion, which had been observed experimentally a decade before. Present findings drawn from the atomic level simulation suggest that the effects of helium bombardment should be taken into account to understand and evaluate the behavior of hydrogen isotopes in the fusion environment.