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Interstitial-mediated diffusion and clustering for transmutation elements Re and Os precipitation in W[1] HONG-BO ZHOU, YU-HAO LI, GUANG-HONG LU, School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China — Under high energy (14 eV) neutrons irradiation in nuclear fusion devoices, tungsten (W) will undergo transmutation to its near-neighbors in the periodic table, such as rhenium (Re), osmium (Os), etc. The transmutation elements Re and Os will precipitate and form new Re/Os-rich phase, and further significantly degrade the mechanical properties of W. Here, we have investigated the mechanism for the irradiation-induced Re/Os clustering in W using the first-principles method and thermodynamic models. It is found that there is strong attraction between Re/Os and self-interstitial atom (SIA) in W. The SIA can be easily trapped by Re/Os once overcoming a low energy barrier, and form W-Re/Os complex dumbbell. The diffusion energy barrier of W-Re/Os is much lower than that of Re/Os diffusing via mono-vacancy or even vacancy clusters. Further, the W-Re/Os can be easily trapped by the substitutional Re/Os atoms, and form high stable Re-Re/Os-Os dumbbell structure. Most importantly, the Re-Re/Os-Os dumbbell can serve as trapping centre for subsequent interstitial-Re/Os, leading to the growth of Re/Os-rich clusters in W. Our finding suggests an interstitial-mediated mechanism for the irradiation-induced Re/Os clustering in W.

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