Carbon clustering and effect on hydrogen trapping in tungsten: First-principles studies

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To understand the effect of carbon (C) on hydrogen (H) behavior in tungsten (W) exposed to succeeding C deposition in fusion reactors, first-principles density functional theory calculations have been performed to evaluate the C clustering in W with and without vacancies and the effect of C content on the H trapping at a vacancy. The calculations were performed in 128-atom and 432-atom supercells. The results show that the nascent formation of W carbide is based on a pair of C atoms located at two neighboring octahedral interstitial sites along the \textit{<111>} direction with a distance of 0.284 nm. Interstitial C atoms prefer to form a zigzag chain between two \{110\} planes, and the C binding energy increases with increasing number of C until four C atoms and then saturates at a nearly constant value of 0.7 eV for larger C clusters. The presence of vacancies enhances the interactions between C and its first nearest neighbor (1NN) W atoms because of strong hybridization between the C-\textit{p} state and \textit{d} state of its 1NN W, strengthening the C trapping at vacancies. Meanwhile, the appearance of C improves the stability of di-vacancy in W. However, the H binding energies to carbon-vacancy-hydrogen (C\textsubscript{m}VH\textsubscript{x-1}) complexes decrease with increasing C contents. For a given C content, the H binding energies to C\textsubscript{m}VH\textsubscript{x-1} complexes generally decrease with increasing number of H. The maximum H content that can be trapped by C\textsubscript{m}V complexes decreases monotonically with increasing number of C atoms, and the C effect on H trapping is dependent on temperature.