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Understanding physical origin of hydrogen/helium and tungsten interaction via an optimal charge density

Professor Guang-Hong Lu

Department of Physics,
Beijing University of Aeronautics and Astronautics

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要旨

Tungsten (W) is considered to be a promising candidate for the first-wall and divertor plate in fusion reactors. He irradiation is one of the key concerns for W PFM and has been under intensive investigations. We reveal the microscopic vacancy trapping mechanism for H bubble formation in W with vacancy defect, which provides an isosurface of optimal charge density that induces collective H binding on its internal surface, a prerequisite for the formation of H_2 molecule and nucleation of H bubble inside the vacancy.

The local lattice expansion induced by the presence of interstitial He atom leads to the local optimal charge density decreasing. This makes interstitial He act as a trapping center for H in W. He-vacancy (He-V) can hold much more H atom than a monovacancy. However, the H trapping energy of He-V complex is lower than that of a monovacancy by 0.18 eV. Significantly, the existence of He can suppress the formation of H_2 in a vacancy, because the prerequisite space for the formation of H_2 molecule is occupied by He. This provides effective approaches to suppress the formation of H bubbles in PFMs.

主催：　東京大学グローバルCOEプログラム「機械システム・イノベーション国際拠点」
本件連絡先：　東京大学大学院工学系研究科マテリアル工学専攻　教授　渡邉聡
E-mail: watanabe@cello.t.u-tokyo.ac.jp　Phone: 03-5841-7135
GCOE事務局　E-mail: gmsi-office@mechasys.jp　Phone: 03-5841-7437