Poster Session | B. Challenges in the Multiscale Modelling of Radiation Effects in Nuclear Materials

[PO-B2]Poster Session 2

Symposium B

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-09]Influence of anisotropic strain and temperature on hydrogen dissolution in tungsten

○Ying zhang[1], Quan Fu Han[1], Yue lin Liu[2], Guang Hong Lu[1] (1.Beihang University, China, 2.Yantai University, China)

Tungsten (W) is an alternative candidate for a plasma facing material in the future fusion reactor due to its high melting point, high thermal conductivity and low plasma sputtering yield. The solubility of hydrogen in tungsten is a basic and crucial factor to influence the formation of hydrogen bubbles. In this work, we have investigated the effects of anisotropic strain and temperature on the dissolution of H in tungsten via the first-principles calculation in combination with thermodynamic models. The temperature and strain effects are reflected by the vibration Helmholtz free energy in the quasi-harmonic approximation and uniaxial/biaxial strain loading, respectively. It is found that the solubility of hydrogen can be enhanced by both compressive and tensile anisotropic strain, independent with of the sign of strain. This is different from the influence of isotropic strain, where the solubility of hydrogen in tungsten responds to the isotropic strain monotonically. Besides, the difference of the dissolution energy between hydrogen dissolves in tetrahedral and octahedral site constantly changes in the anisotropic strain range of -4%-4%. Further, under same anisotropic strain condition, the solution energy of hydrogen in tungsten increases with the increasing of the temperature from 300-1800 K, which can be mainly contributed to the vibration Helmholtz free energy. Our finding suggests that the local anisotropic strain and temperature can significantly influence the dissolution of hydrogen in tungsten, which may play a key role on hydrogen bubble formation.