Critical Concentration for Hydrogen Bubble Formation in Tungsten

L. Sun\textsuperscript{a}, S. Jin\textsuperscript{a}, H. B. Zhou\textsuperscript{a}, Y. Zhang\textsuperscript{a}, G. H. Lu\textsuperscript{a}, X. L. Shu\textsuperscript{a}, W. Zhang\textsuperscript{b}, H. T. Lee\textsuperscript{c} and Y. Ueda\textsuperscript{c}

\textsuperscript{a}School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China
\textsuperscript{b}Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China
\textsuperscript{c}Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan

jinshuo@buaa.edu.cn

In the fusion devices, tungsten (W) will be exposed to high fluxes of H isotopes, leading to unexpected surface blistering. The local H concentration is believed to directly affect the formation process of H bubble, and thus play a critical role in determining the property degradation and mechanical integrity of W.

Using the energetics of H calculated from first principles as input parameters, we are able to determine the H concentration in metals such as W via the thermodynamic models. For H concentration in intrinsic metals without any defects, such thermodynamic model has been well established as the well-known Sievert’s law. It is more practical, however, to determine the H concentration in metals with defects such as a vacancy. With the consideration of defects in W, we further derive formulations of the thermodynamic model that are more suitable for vacancy and multiple H-vacancy complex. Based on the derived formulations, we calculate the equilibrium H concentration and its dependence on the H pressure and temperature using the first-principles dissolution energies for W as inputs [1].

At a certain temperature, the H concentration exhibits a sharp increase beyond a critical H pressure, which is mostly originated from the increase of H at the mH-V complexes. This indeed corresponds to a critical H concentration associated with the H bubble formation in W. Such critical concentration and pressure are clearly defined as the values when the concentration of H at one certain mH-vacancy complex first equals to that of H at the interstitial, which are 24 ppm/7.3 GPa at 600 K in W. Beyond such critical H concentration, considerable H atoms will accumulate into the vacancy, leading to the formation and rapid growth of the H-vacancy complexes, which is the preliminary stage of the H bubble formation. Consequently, we are able to plot a pressure-temperature phase diagram for W with and without H bubble formation separated by the critical H concentration as a function of temperature.

Experimentally, the ion-driven H isotope permeation in W has been investigated using a high flux ion beam test device coupled with a permeation device [2]. This gives clear information whether the H bubble forms for the measured H concentration points based on the Zakharov’s diffusivity. The experimental H concentrations are within the predicted phase region by the thermodynamics model both with and without H bubble formation. This suggests that the predicted critical H concentrations are consistent with experimental observations, and thus may serve as a possible criterion to evaluate the H induced failure of metallic PFM's in the future fusion reactors.