Background

- The degradation of mechanical properties, due to the accumulation of hydrogen isotopes in the materials, is enhanced by the existence of defects
- The retention of tritium in plasma facing component is a key issue related to the safety and economics
- It is indispensable to study the transport of hydrogen in the materials with defects
- The transport of hydrogen in the materials with vacancies is less understood

Objective

Study the Influence of hydrogen-vacancy interaction on the mobility of hydrogen and vacancy in bcc-metal

1. Influence of H-V interaction on the mobility of H

1.1 Diffusivity of H in different systems (MD)

- The diffusivity of H is decreased due to the interaction with V
- With H/V ratio increasing, the diffusivity of H increases
- Similar diffusivities are observed in the same H/V-ratio systems, except for V1-H1 and V8-H8
- V1-H1 system: no other H atom is mobile in the bulk while the sole H is trapped by V

1.2 Model to evaluate the effective diffusivity of H

- For comparison: Fe342-H1, Fe431-V1
- Temperature: 700, 800, 900 and 1000 K
- Simulation time: 0.2 fs/step, 6×105 step (12 ns)

Einstein diffusivity equation

\[ D = \lim_{t \to \infty} \frac{1}{6Nt} \sum_{i=1}^{N} (r_i(t) - r_i(0))^2 \]  

MSD/6 for hydrogen

Diffusivity of vacancy

Decay of fraction of non-trapped-H

Fraction of non-trapped-H

Diffusivity of H (MD VS. Model)

T-site

O-site

\[ f_{\text{non-trapped}} + f_{\text{trapped}} = 1 \]

\[ D_{\text{eff}} = D_{\text{trapped-H}} \times f_{\text{trapped-H}} + D_{\text{non-trapped-H}} \times f_{\text{non-trapped-H}} \]

Fitted by counting the number of hydrogen atoms located away from the vacancy more than 0.6Å (MD)

Diffusivity of H in Fe342-H1 system (D_{eff})

\[ D_{\text{eff}} \approx D_H \times f_{\text{non-trapped}} \]

\[ f_{\text{non-trapped}} \times D_H = D_{\text{eff}} \]

2. Influence of H-V interaction on the mobility of V

Diffusivity of V in different systems

Different V configurations (V8-H8)

- The diffusivity of V is decreased due to the H-V interaction
- Except V1-H1 system, with H/V ratio increasing, the diffusivity of V increases

Summary

- The diffusivity of H is obviously decreased due to the H-V interaction when they co-exist in the system
- With H/V ratio increasing, the fraction of non-trapped-H increases, which induces the diffusivity of H increasing
- A simple model to evaluate the effective diffusivity of H in the system with V is proposed
- The mobility of V (isolated) is decreased due to the H-V interaction when they co-exist in the system
- The clustering of V obviously decreases the mobility of V, but has no significant influence on the mobility of H

Influence of V clustering on the mobility of V and H

MD for iron

Diffusivity of H (10^-8 m^2 s^-1 900 K)

V8H8

0.59

0.60

V8H48

1.53

1.56

The clustering of V does not significantly influence the mobility of H