# Influence of H-V interaction on the mobility of H and V in bcc-metal

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## 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

### **Research method**

- ✓ Modelling material:  $\alpha$ -iron
- Reliable potential model [1] of the embedded atom method (EAM) is available regarding the interaction with hydrogen
- $\circ$  Similar bcc structures and similar hydrogen trapping behaviors in  $\alpha$ -iron and tungsten
- ✓ Molecular Statistics (MS) and Molecular dynamics (MD) simulation: LAMMPS code

System	V conc. (at.%)	Supercell	H conc. (at.%)	H/V ratio
Fe431-V1-H12	0.231	6×6×6	2.78	12
Fe431-V1-H6	0.231	6×6×6	1.39	6
Fe431-V1-H3	0.231	6×6×6	0.694	3
Fe431-V1-H1	0.231	6×6×6	0.231	1

#### **Einstein diffusivity equation**

- For comparison: Fe432-H1, Fe431-V1
- Temperature: 700, 800, 900 and 1000 K
- Simulation time: 0.2 fs/step, 6×10<sup>7</sup> step (12 ns)



✓ 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)** 



**1.2 Model to evaluate the effective diffusivity of H** 



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



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 Ο