**Background**

- The formation of fiber-like nanostructures on tungsten (W) and molybdenum (Mo) are observed after helium (He) plasma exposure.
- Their formation mechanism has not been understood well.
- The He bubble seems to have a influence on these nanostructures.

**Purpose**

1. To investigate microscopic relationship between metal and He bubble
   - Calculate variations of He binding energies using first principle calculation based on density functional theory (DFT)
2. To expand macroscopic simulation from DFT calculation results
   - Developed He diffusion / aggregation simulation code based on kinetic Monte Carlo method (KMC)
   - Investigate differences in formation of bubbles for each metal by KMC simulation

In this study, KMC simulation is performed on interstitial sites of bcc metal, which does not consider vacancy.

**Results of DFT calculation**

**Definition of He bind energy**

\[
E_{bind}^n(z) = E_{tot}(Mo, He_z) - E_{tot}(Mo) + E_{vac}(Mo, He_{z-1}) + E_{vac}(Mo, He_{z-2})
\]

The binding energies at interstitial sites

- A metal with monovacancies has a higher binding energy
- A fiber-like nanostructure formable metal has a higher binding energy
- The peak position of the graph depends on the crystal structure

**He bubble formation at each temperature in BCC metal's calculated by KMC simulation**

**Simulation condition**

- Box size: 30 x 30 x 30 unit cells
- Periodic boundary
- He/W: 0.01
- The number of helium does not change over time
- Elapsed time: 1µs
- The initial position of helium is randomly arranged at the T-site of each metal
- Diffusion coefficient:
  - \(3.36 \times 10^{-8} \exp(\frac{\Delta E_{0}}{k_B T})\)

**Average number of connection per elapsed time**

- **Temperature dependence (W)**
  - **Metal dependence (500 K)**

**He connection model in KMC**

- Single He atom in BCC metal passes through the migration path on the right side and is trapped at the T-site
- In DFT calculation, He tends to be trapped more easily at the T-site than the D-site when aggregated between the lattices and He is likely to be trapped in the vicinity of the second nearest T-site when viewed from the other He
- In this KMC model, He jumps only between T-sites and is regarded as connecting when He is adjacent to the second nearest T-site.

**How to obtain \(\Delta E_{connect}\) from DFT calculation result**

- We want to express \(\Delta E_{connect}\) as a function of a certain number \(k\) of connections with another He.
- If there is a cluster of \(n\) helium, the total energy that the cluster has \(E_{total}\) is
  \(E_{total} = E_{gas}(z) = E_{gas}(1) + 2E(2) + 3E(3)\)
- Fitting \(E_{gas}(n)\) in the form of \(a + b n^k\)

**He diffusion: T-site**

**KMC calculation method**

- What is KMC:
  - A method to make statistical behavior by repeating the particle jumping randomly between lattices with certain event
- What is KMC's event in this research:
  - One helium at a certain T-site moves to some neighboring T-site
  - The probability \(P_i\) that an event \(i\) occurs
    \(P_i = P_0 \exp(-\frac{\Delta E_{i}}{k_B T})\) [s\(^{-1}\)]
  - A migration barrier energy \(\Delta E_{migration}\) that a certain He does not connect to other He
    \(\Delta E_{migration} = \Delta E_0\)
  - A daretrop barrier energy \(\Delta E_{daretrop}\) that a certain He is connected to k other He
    \(\Delta E_{daretrop} = \Delta E_{migration} + \Delta E_{connect}\)
  - \(\Delta E_0\) and \(\Delta E_{connect}\) are obtained by DFT

**Summary**

- By comparison between DFT calculation and experimental results, fiber-like nanostructures tend to be formed with metals with a higher binding energy
- In order to investigate the relationship between the DFT calculation results and the He bubble formation tendency, we developed He aggregation / diffusion simulation code based on KMC.
- Temperature and material dependence of He bubble formation was observed by KMC simulation and there is an appropriate temperature range for the bubble growth.
- Large bubbles are formed at temperatures as high as 1000 K or more for W and Mo with higher binding energy obtained by DFT