A KMC Simulation of Grain Size Effects on Bubble Growth and Gas Release of Implanted Tungsten

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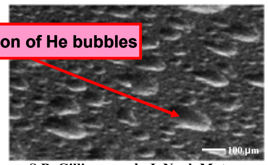
Motivation and Objective

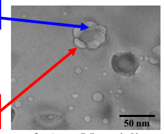
- **High irradiation environment**
  - First wall of fast breeder reactor
  - First wall of nuclear fusion reactor
- **Formation of helium bubble**
  - Segregation around grain boundaries
  - Swelling of the material
- **ODS (Oxide Dispersion Strengthened) steel**
  - Possible to use under elevated temperatures
  - Low swelling
    → Experimental observation

Y_2O_3 particles capture the Helium bubbles

Modeling of Helium bubble diffusion in the material



S.B. Gilliam, *et al.*, J. Nucl. Mater., 347, (2005), 289-297



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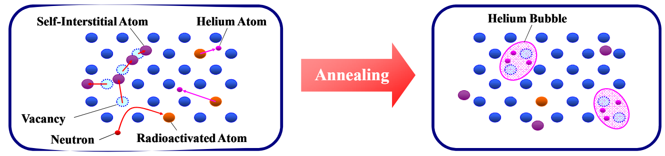
Modeling of Helium Bubble

- **Formation of helium bubbles**



- Helium bubbles are produced by
- The diffusion of helium bubbles and vacancies generates helium bubbles

- **Modeling of helium bubble**

Ideal gas law: $PV = nkT$

Young-Laplace equation : $P = 2\gamma / r$

Assume spherical bubbles: $V = 4\pi r^3 / 3$

P : Internal pressure
r : Radius of bubbles
n : Number of atoms
k : Boltzmann constant
T : Temperature
γ : Surface energy
V : Volume of bubble

Delete P →

Radius of bubble: $r = \left(\dfrac{3nkT}{8\pi\gamma} \right)^{1/2}$

KMC Simulation of Helium Bubble Diffusion in a Polycrystal

- **KMC method**
  - **Frequency of diffusion event**

$$\nu = \nu_0 \exp\left(\frac{-E}{kT} \right)$$

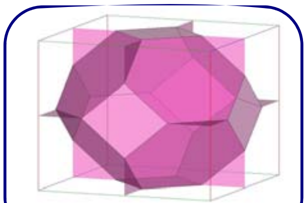
k : Boltzmann constant
ν_0 : Pre-factor
T : Temperature
E : Activation energy

  - **Time step**

$$\Delta t = \frac{-\log R}{\sum_i \nu_i}$$

ν : Frequency
R : Random number

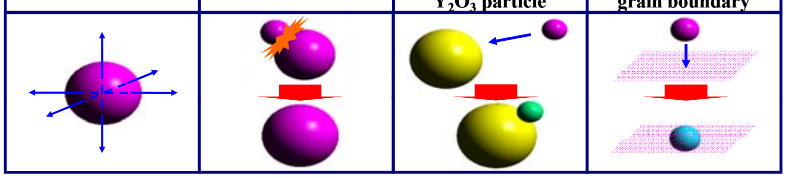
- **Shape of crystal grains**



Truncated Octahedron

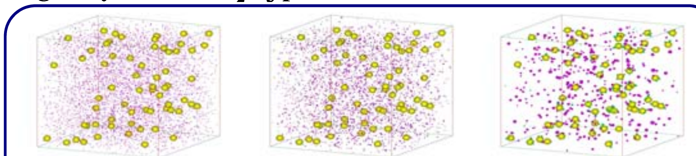
- **Possible events in the KMC simulation**

Diffusion	Clustering	Captured by Y_2O_3 particle	Captured by grain boundary



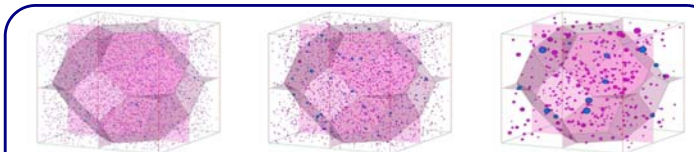
KMC Simulation Results (Helium Bubble Diffusions)

- **Single crystal with Y_2O_3 particles**



10^2 [s] 10^4 [s] 10^6 [s]

- **Polycrystal without Y_2O_3 particles**



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: helium bubble
: Y_2O_3 particle
: helium bubble caught by Y_2O_3 particles
: helium bubble caught by grain boundary

KMC Simulation Results for Polycrystalline ODS Steel

- **Analysis condition**

Simulation volume	500×500×500[nm³]
Boundary condition	Periodic
Temperature	500[℃]
# of bubbles	5000
Diameter of bubble	3[nm]
Number density of Y_2O_3	* 5.10×10²⁰[m⁻³]

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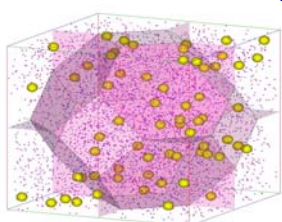
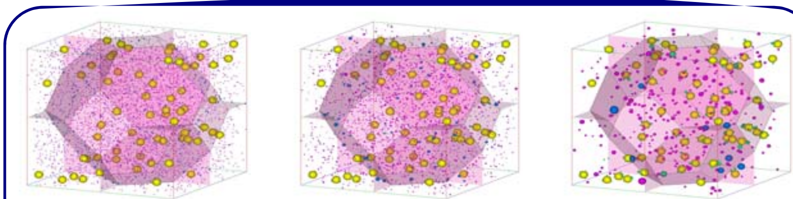


- **Helium bubble diffusion behavior**



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- **Influence of Y_2O_3 particles and grain boundaries**