First Principles Modeling on Radiation Defects in W and W-based Alloys

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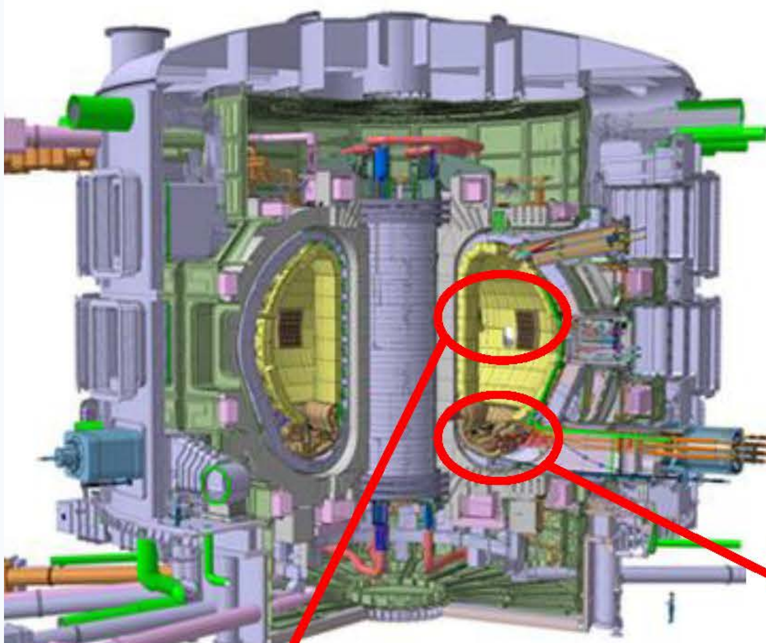
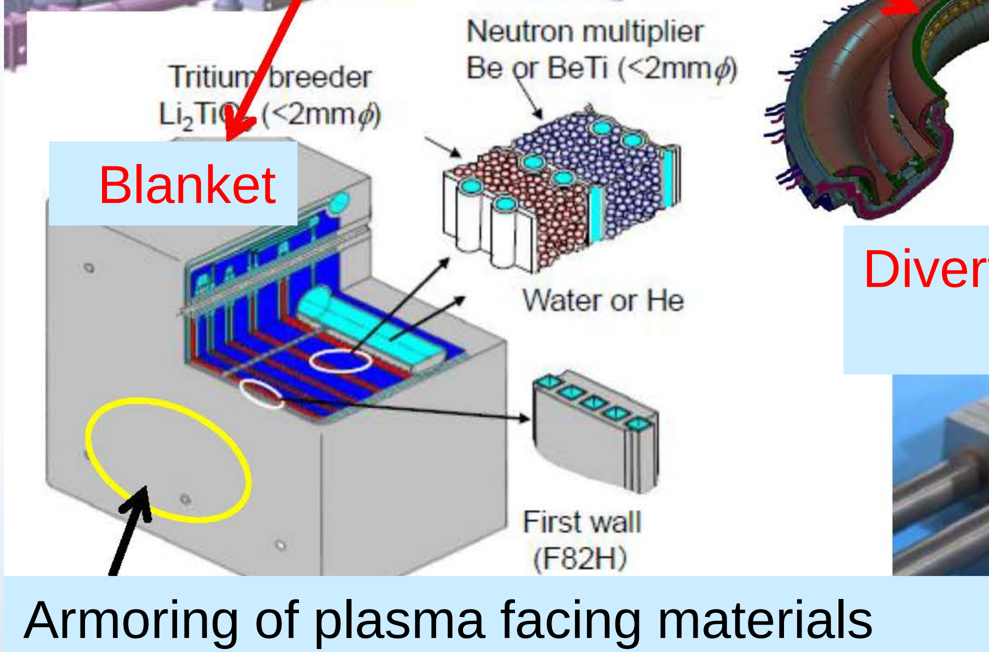
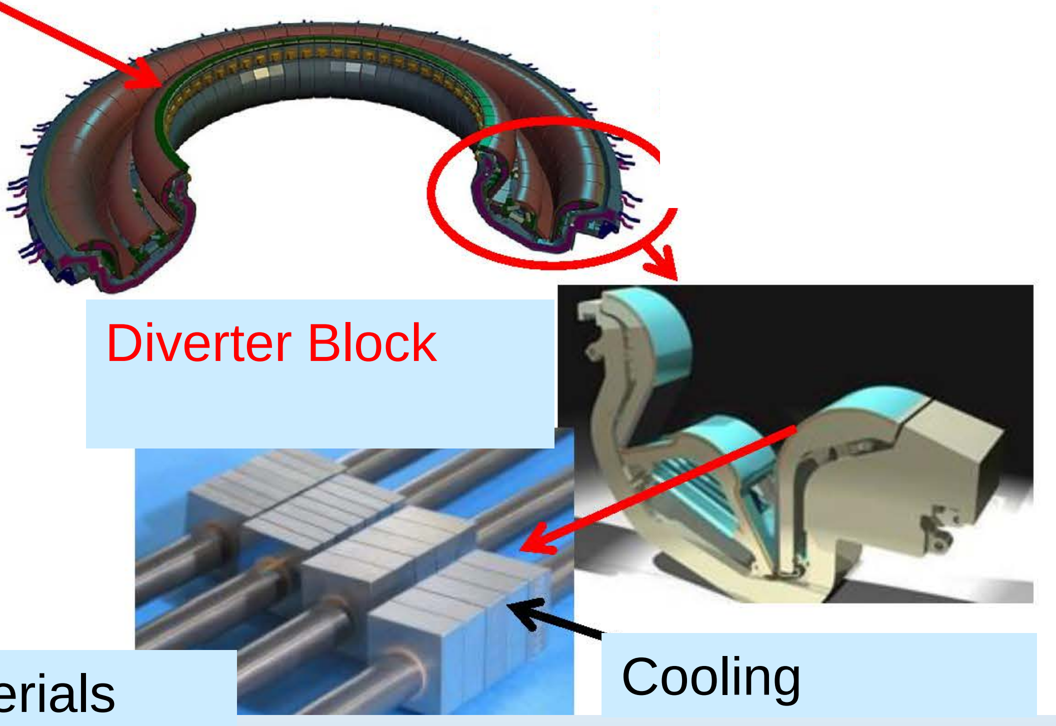
Application of tungsten to nuclear fusion reactor

- High melting point
- High resistance to spattering
- Low hydrogen absorption

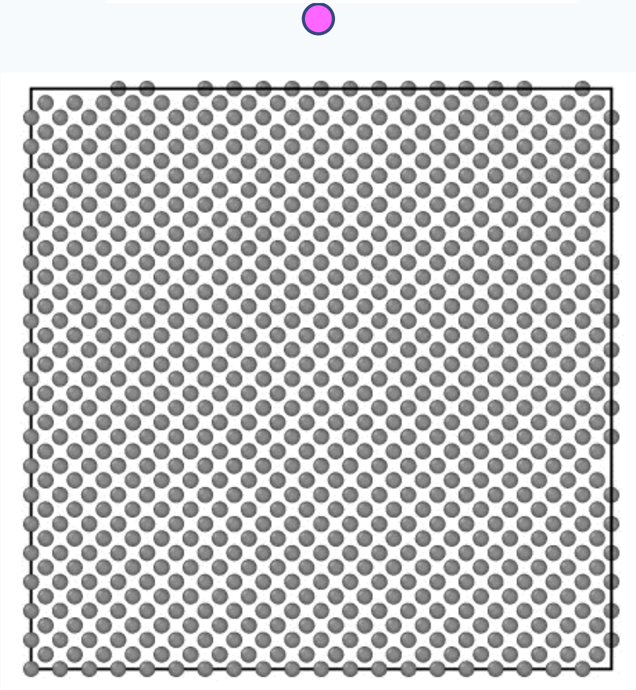


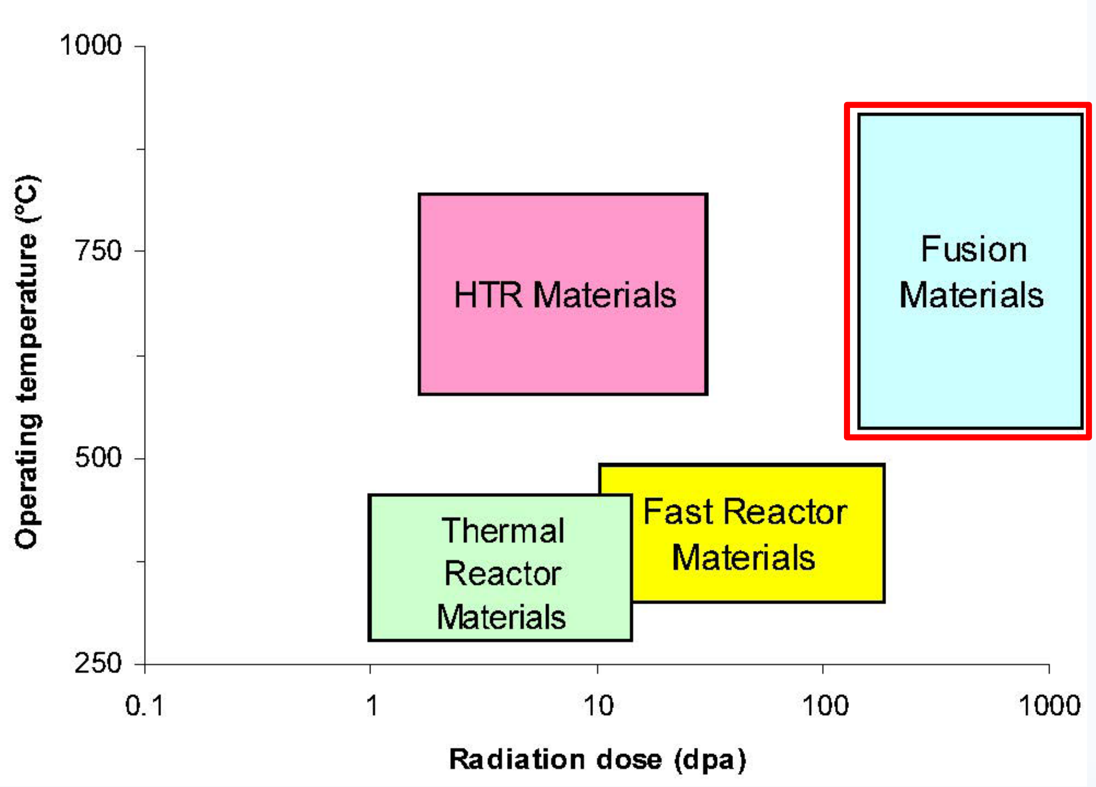




Irradiation to fusion materials is severe

High-energy particle





Molecular dynamics by LAMMPS (BCC Fe)

Operational condition of materials in various nuclear devices (IAEA GC51)

Neutron irradiation to W causes Re (and Os) through nuclear transmutation

Nuclear reaction of W under neutron irradiation

$$^{186}\mathrm{W}(n,\gamma)^{187}\mathrm{W}$$

$$\rightarrow(\beta-)\ ^{187}\mathrm{Re}\begin{cases}(n,\gamma)^{188m}\mathrm{Re}\rightarrow(\gamma)\ ^{188}\mathrm{Re}\rightarrow(\beta)\ ^{188}\mathrm{Os}\\(n,2n)^{186}\mathrm{Re}\rightarrow(\beta-)\ ^{186}\mathrm{Os}\end{cases}$$

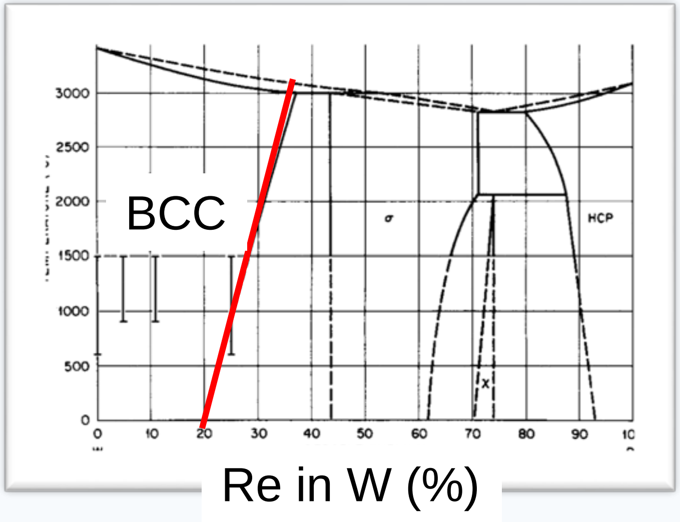
$$^{184}\mathrm{W}(n,\gamma)^{185}\mathrm{W}\rightarrow(\beta-)\ ^{185}\mathrm{Re}(n,\gamma)^{186}\mathrm{Re}\rightarrow(\beta-)\ ^{186}\mathrm{Os}\ .$$

Pure W → W-6Re-3Os (end-of-service)

Cottrrel et al., Fusion Sci. Technol. 50(2006) 89.

Re causes radiation-induced precipitation in W

W-Re phase diagram [1]



Solubility limit of Re > 20%

Neutron-irradiated W-5Re 1.54dpa, 750°C [2]

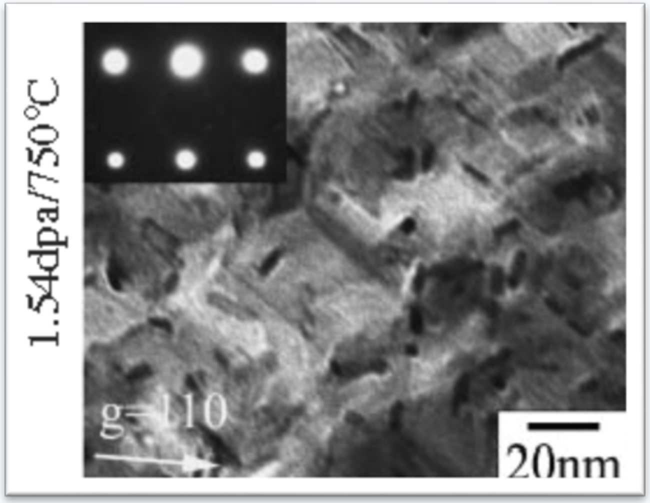
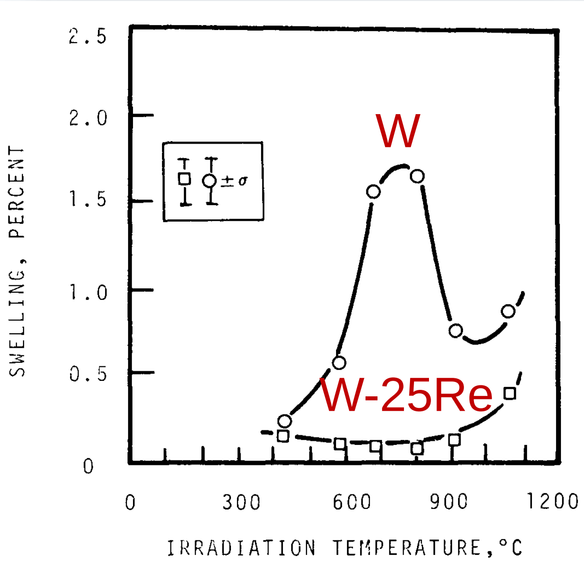


Plate-like or needle-like precipitates (χ-phase, Re_3W)

[1] Williams et al., Metallurgical Trans. A , 14A 655-666(1983)
[2] Tanno et al., Mater. Trans. 49[10], 2259-2264(2008)

Re in W reduce radiation-induced void swelling

Neutron irradiation
9.5 dpa, @EBR-II [1]



Neutron irradiation
1.54dpa, 750℃@JOYO [2]

	W	W-5Re	W-10Re
Void			
Mean diameter [nm]	4.7	3.3	1.6
Density [$10^{22}/m^3$]	12	0.65	3.1
Swelling [%]	0.72	0.01	0.01
Precipitate			
Mean length [nm]	–	14	9.5
Density [$10^{22}/m^3$]	–	7.3	42
Volume [%]	–	1.5	3.6

[1] J. Matolich et al, Scr. Metall. 8 (1974) 837-841.
[2] T. Tanno et al., Mater. Trans. 49 (2008) 2259-2264.

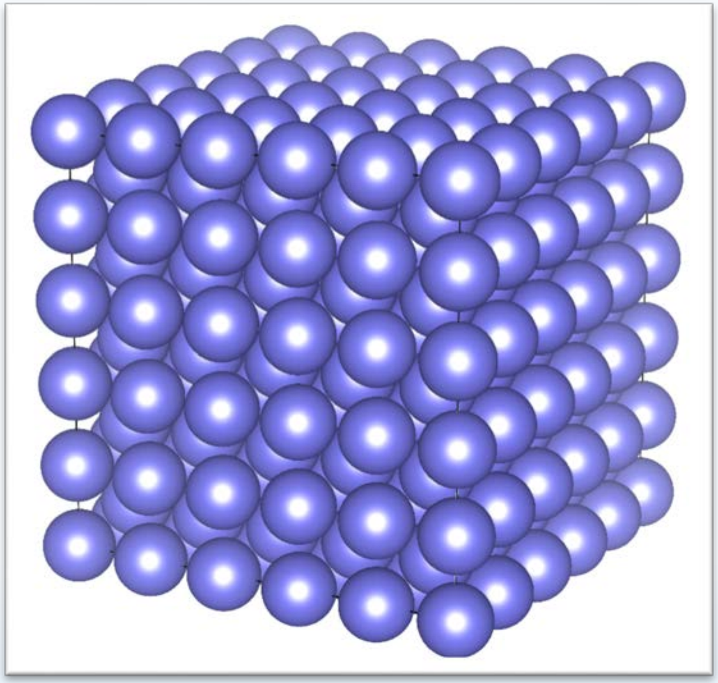
Goal of this study is :

To explain the experimentally-discovered Re-effects using the first-principles calculations

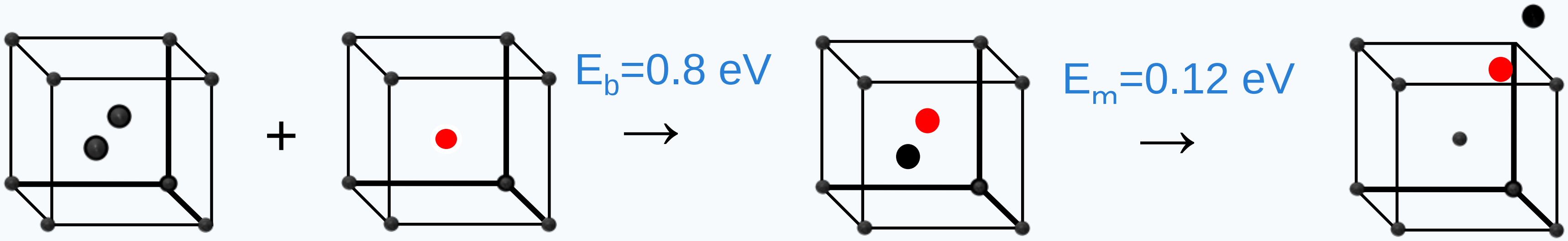
Modeling methodology

- VASP（Vienna *ab initio* Simulation Package）
- Projected augmented wave potential (PAW/PBE)
- $5a_0 \times 5a_0 \times 5a_0$ (250 lattice sites) super cell
- K-point (3×3×3)
- Cutoff energy: 350eV
- Nudged elastic band method to calculate migration barrier

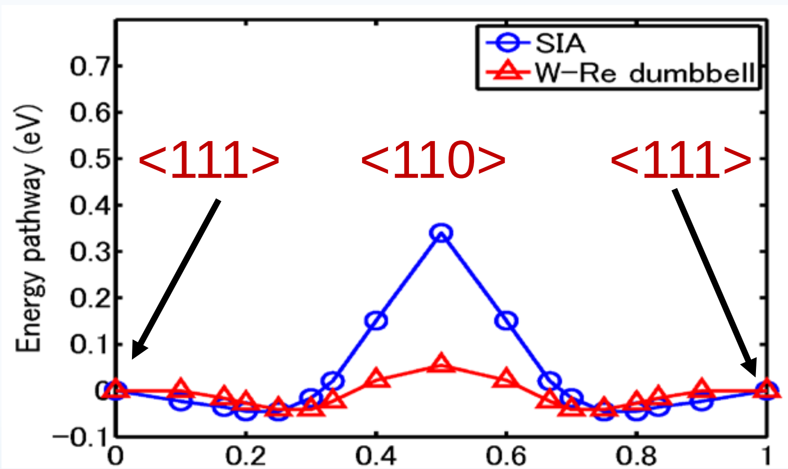
Used super cell

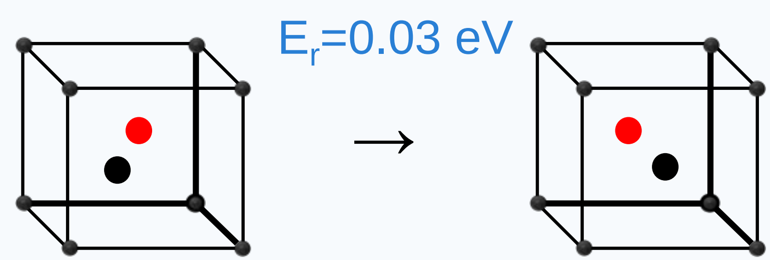


Displaced W forms W-Re dumbbell, which migrate and rotate



W-Re dumbbell can rotate easily

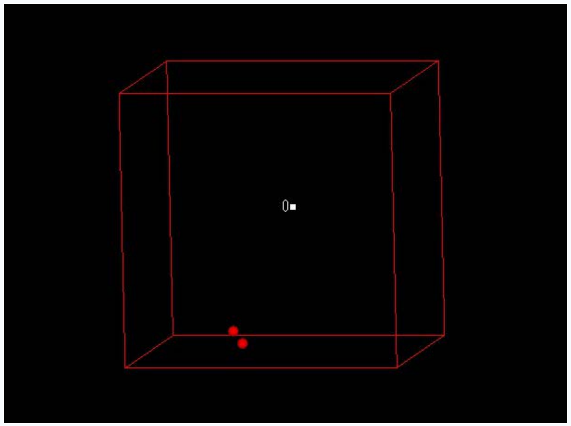




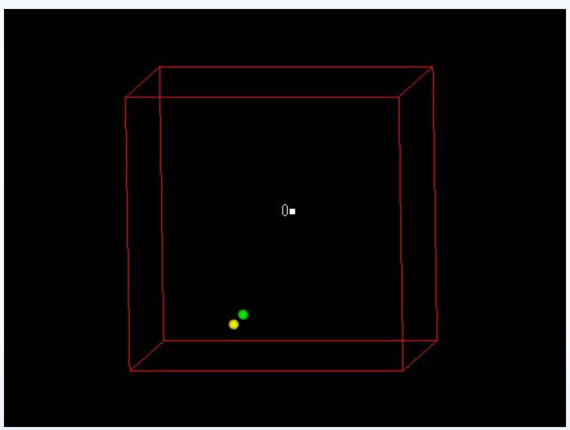
T. Suzudo, M. Yamaguchi, A. Hasegawa, Modeling Simulation Mater. Sci. Eng. 22 (2014) 075006.

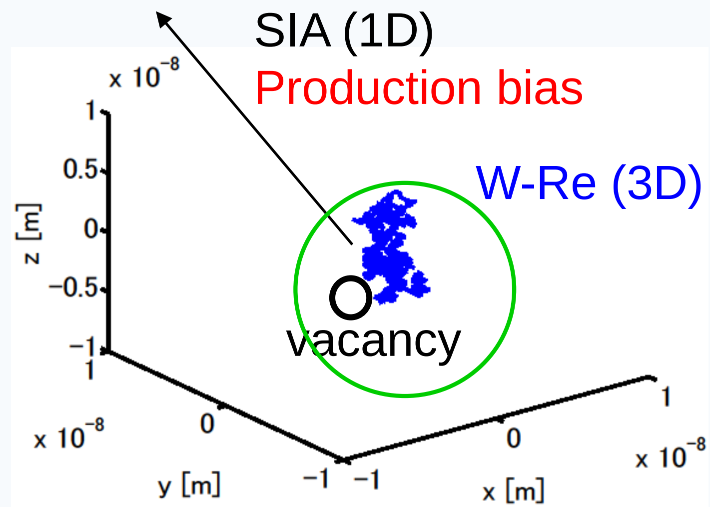
KMC simulation (PAKSS) of 1D SIA and 3D W-Re dumbbell

SIA



Mixed dumbbell





Our results suggest:

- SIA (1D migration)
  → Accumulation of vacancies
- Mixed (3D migration)
  → Enhanced recombination to vacancy
  → Suppression of radiation swelling

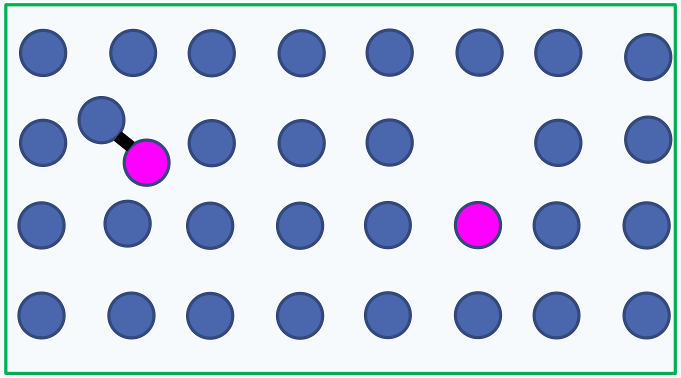
T. Suzudo, A. Hasegawa, Scientific Reports vol. 6, 36738 (2016).

Enhanced recombination also explains the precipitation.

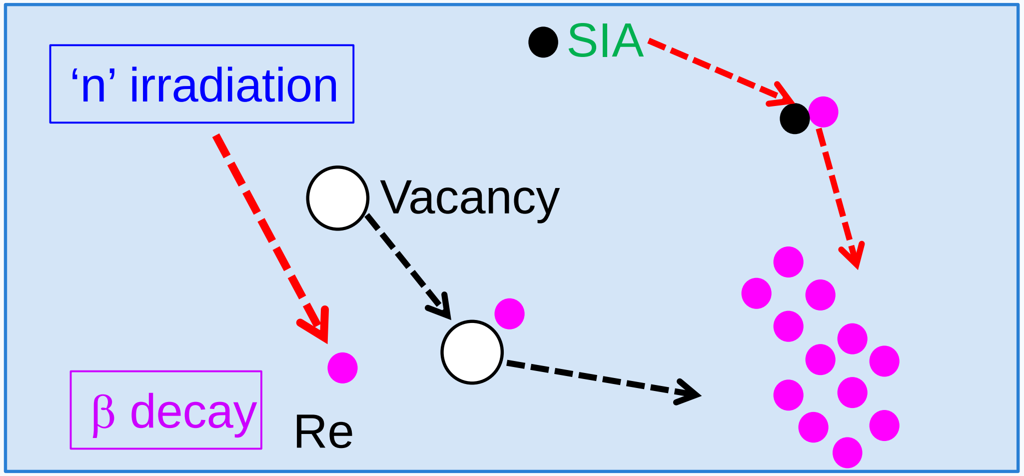
Binding energy

	Vacancy (eV)	SIA (eV)
Re	0.22	0.79

Vacancy and SIA bind Re



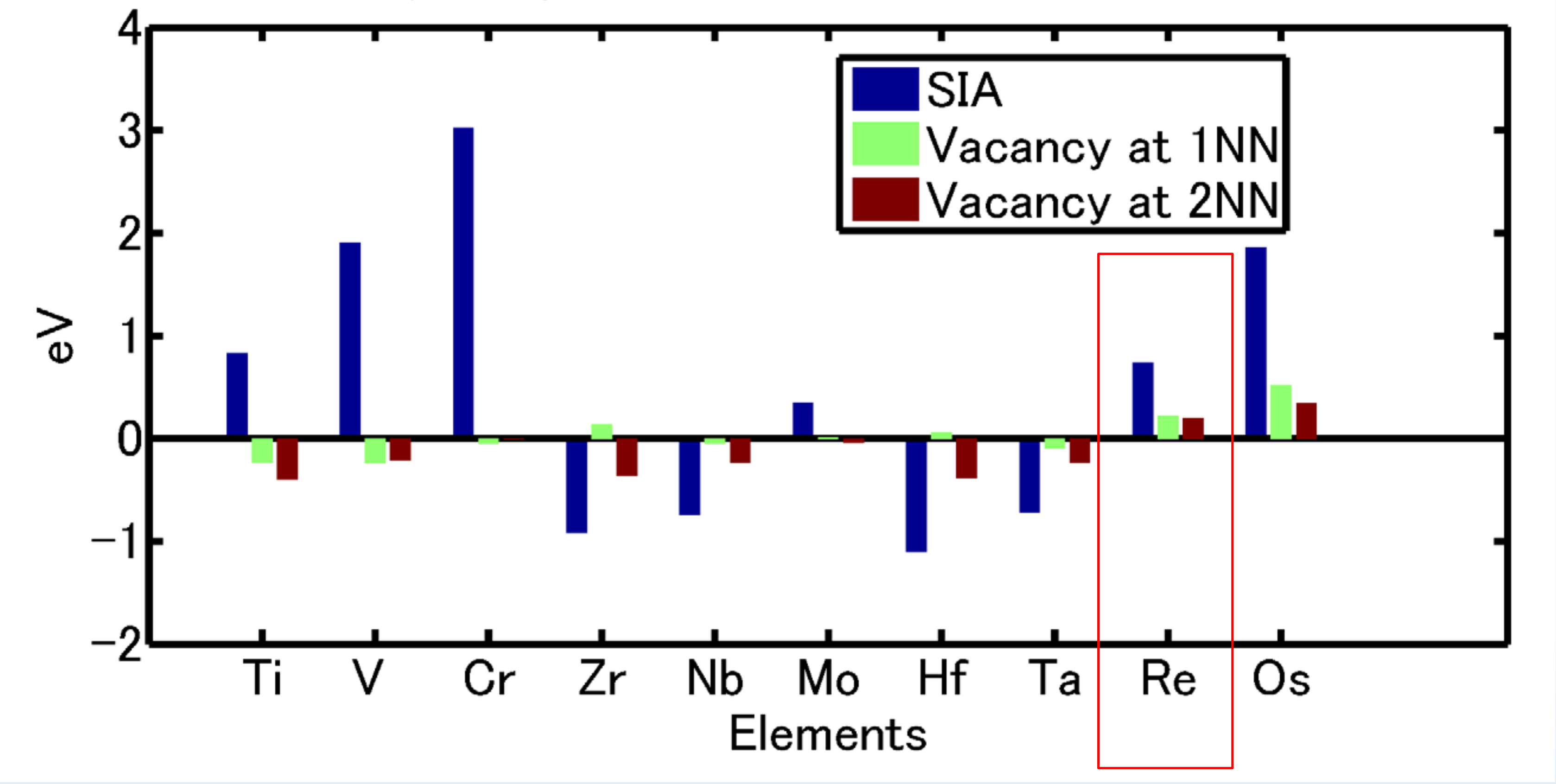
Re atoms are dragged by vacancy and SIA and aggregated through recombination.



Our recombination scenario explains both radiation-induced precipitation and suppression of swelling.

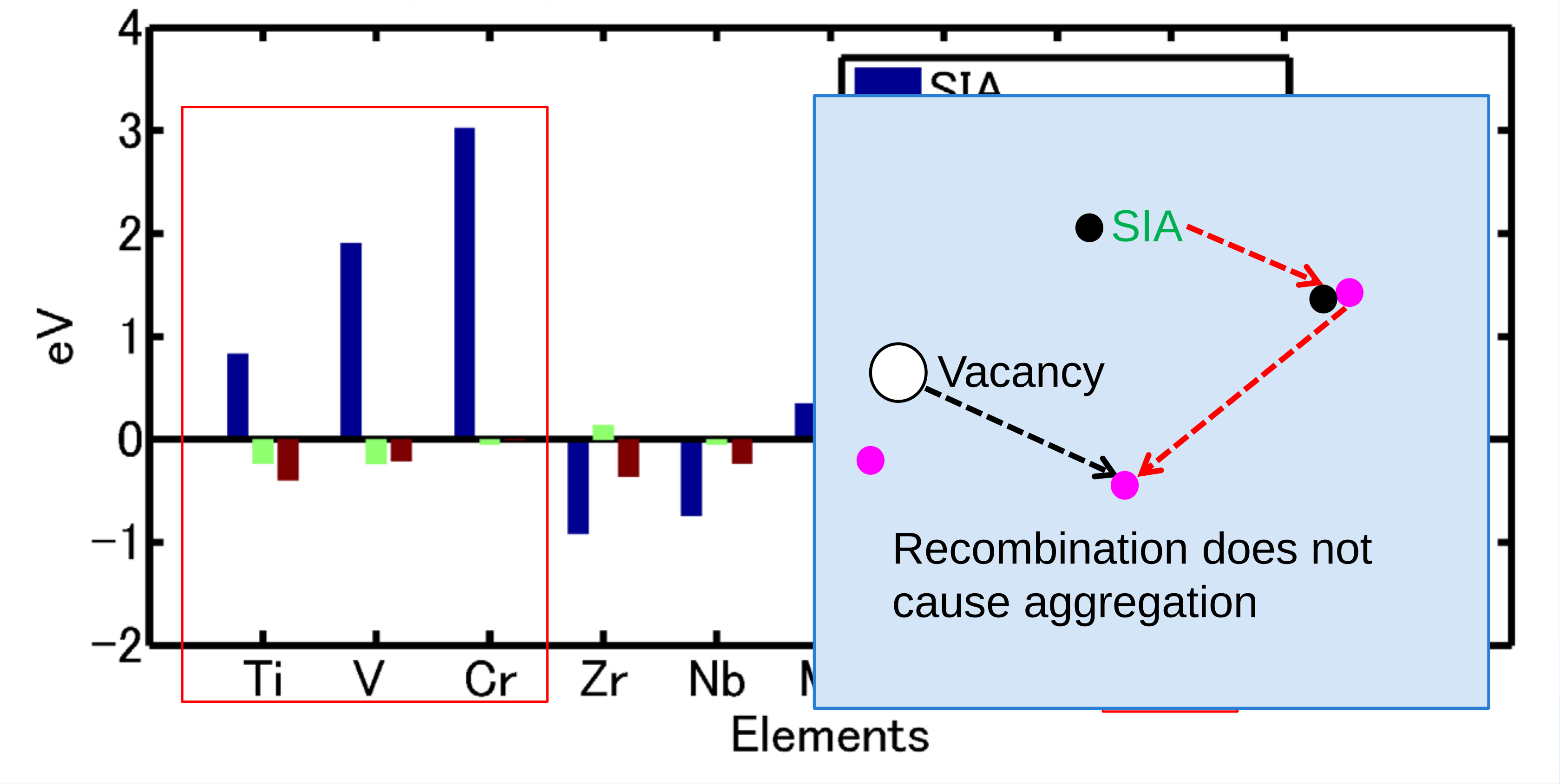
Binding energy for other solute atoms are calculated

Binding energy of solute elements and SIA/vacancy



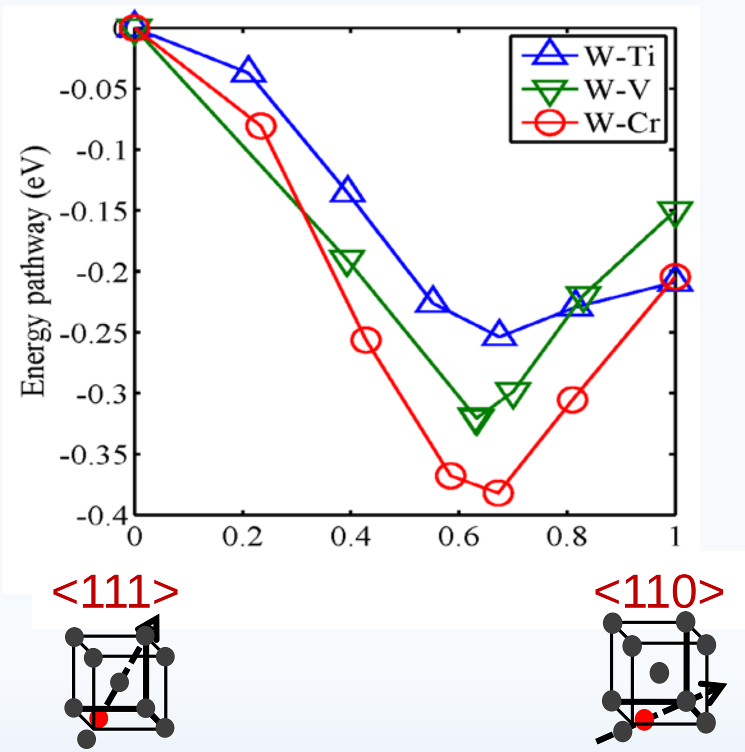
Ti, V, and Cr form mixed-dumbbells, but not solute-vacancy complex

Binding energy of solute elements and SIA/vacancy

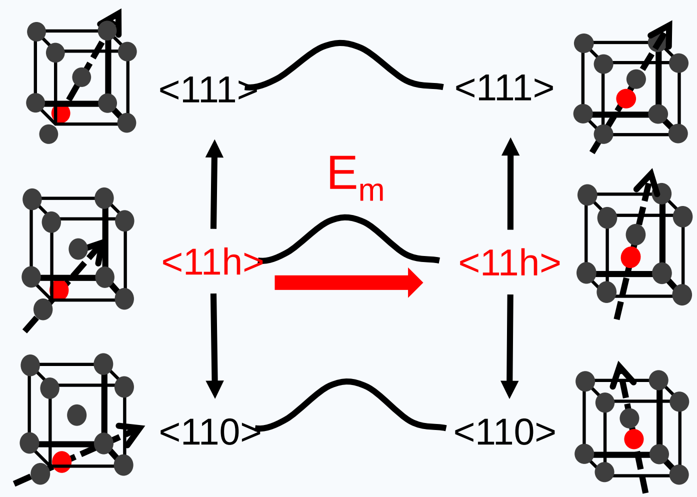


W-Ti, W-V, W-Cr dumbbells also Have 3D motion

<11h> dumbbell is the most favorable
The rotation is easy.



Migration energy of
mixed dumbbell



E_m=0.15 eV for Ti
=0.13 eV for V
=0.12 eV for Cr

T. Suzudo, T. Tsuru, A. Hasegawa, J. Nucl. Mater. 505 (2018) 15-21

Summary

- DFT study predicts 3D migration of W-Re mixed dumbbell, this seems a cause of swelling suppression and radiation-induced precipitation.
- Ti, V, Cr may suppress radiation effect without causing precipitate, but experimental verification is required.