Migration of rhenium and osmium in tungsten

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Neutron irradiation to W causes Re and Os through nuclear transmutation

Principal transmutation path for W

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

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

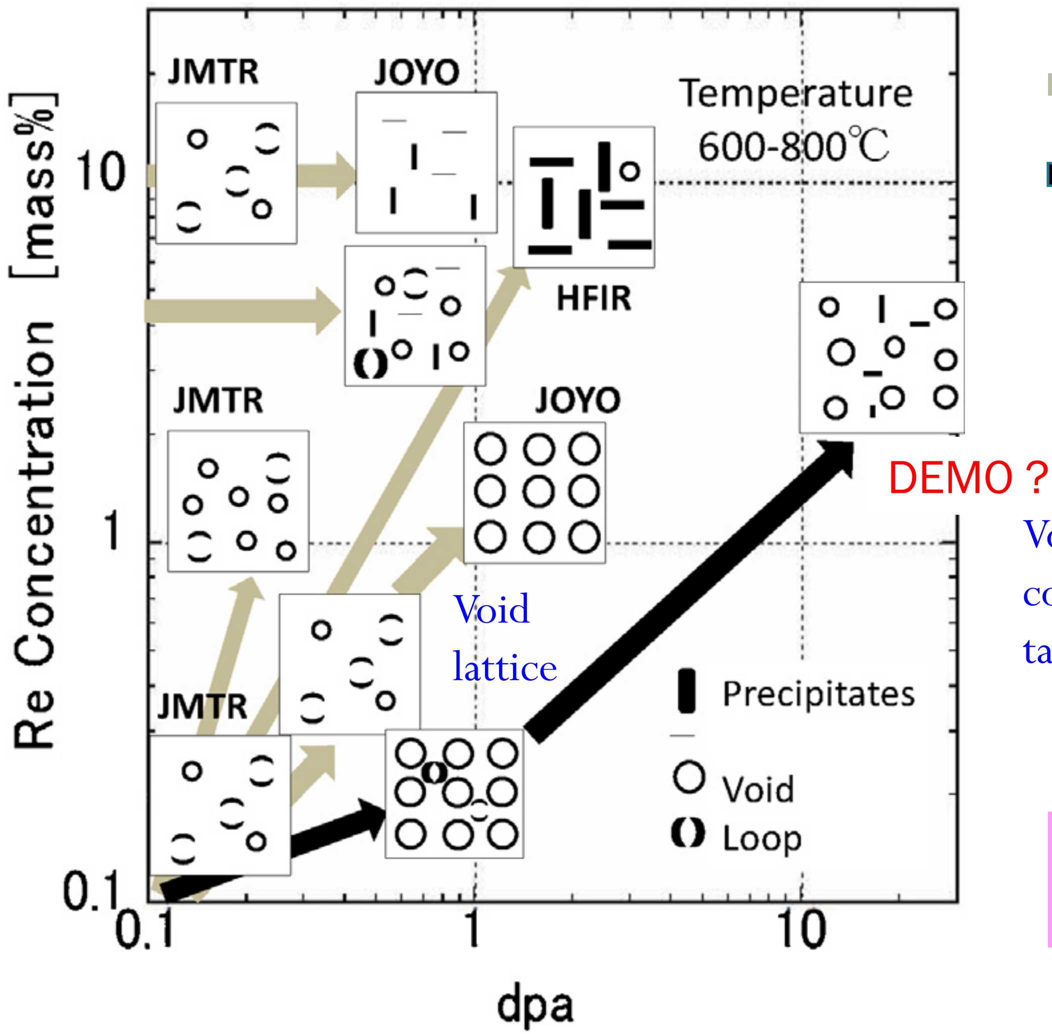
$$^{184}\mathrm{W}(n,\gamma)^{185}\mathrm{W}\rightarrow(\beta-)\ ^{185}\mathrm{Re}(n,\gamma)^{186}\mathrm{Re}\rightarrow(\beta-)\ ^{186}\mathrm{Os}\ .$$

Pure W → (at the first wall) → W-18Re-3Os* (50dpa)

Pure W → W-6Re-3Os** (end-of-service)

*Noda et al., JNM 258-263(1998) 934-939.
**Cottrrel et al., Fusion Sci. Technol. 50(2006) 89.

Microstructure evolution of W-Re under neutron radiation environment*



Observed

Expected in DEMO Condition

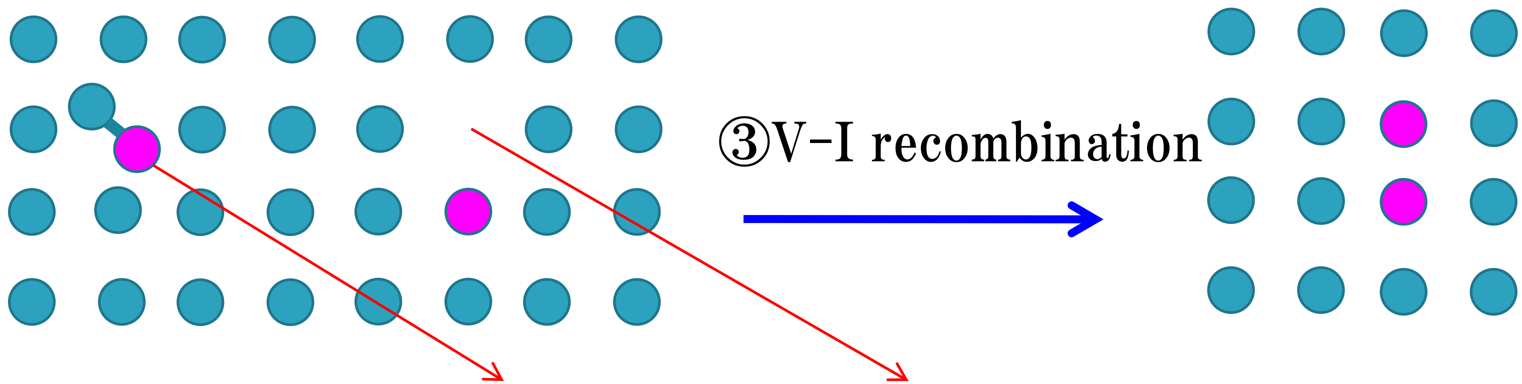
*Hasegawa et al., Fusion Engineering and Design, 89 (2014) 1568–1572

Void lattice may collapse, and RIP takes place?

Establishing a quantitative model is essential.

RIP development mechanism

How solute atoms are aggregated . (J. Martin, Phys. Rev. B 21 (1980) 2121)

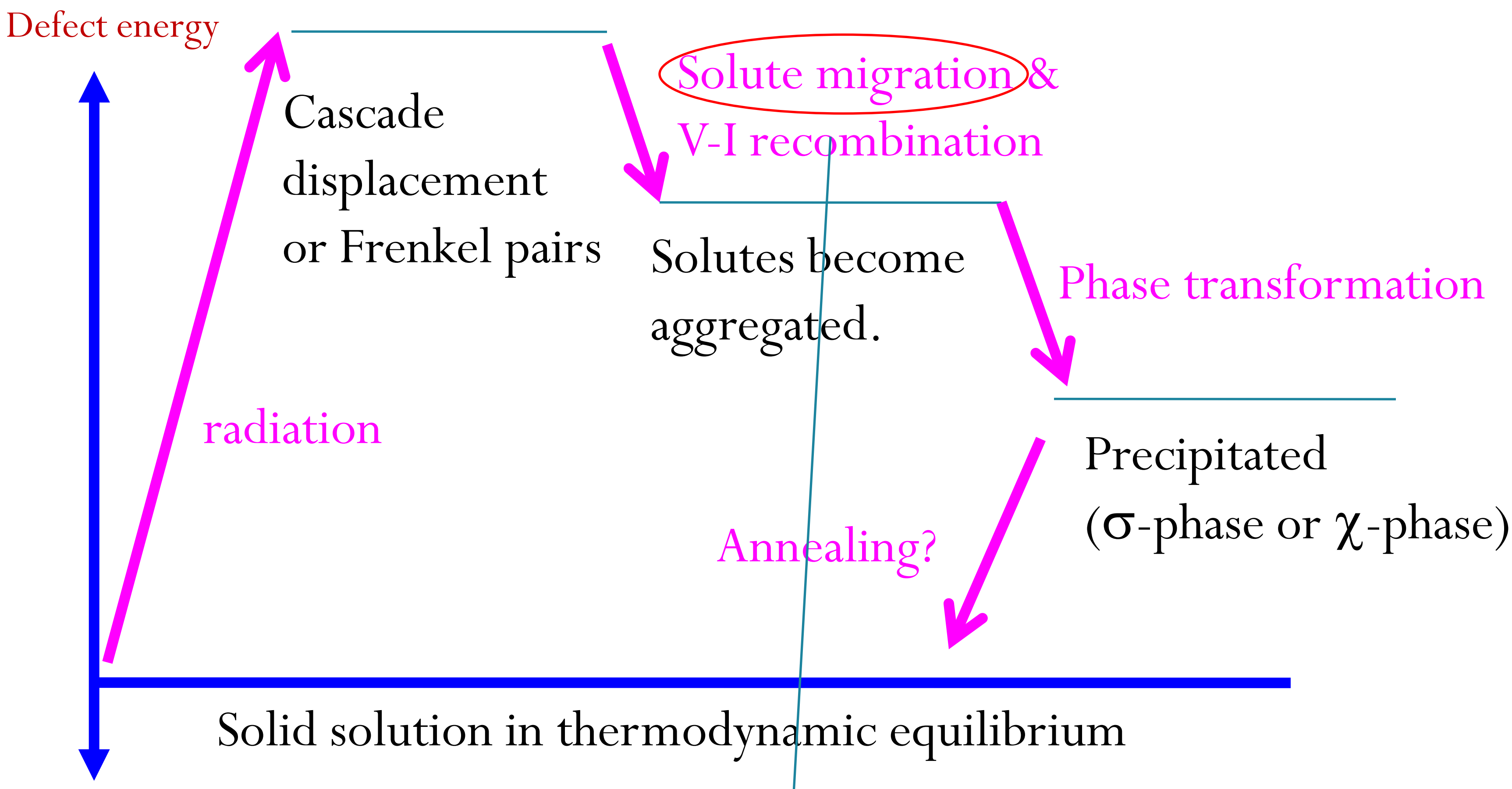


Solute atom is bonded to ①SIA and ② vacancy

Condition for RIP development
① SIA and solute atom must be attractive.
② Vacancy and solute atom must be attractive.
③ Solute atoms must be dragged by SIA or vacancy.

Detailed mechanism of ③ is not known.

Solute migration is essential for RIP

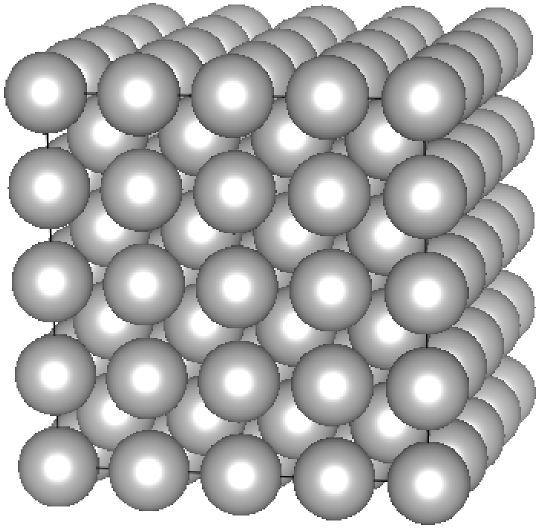


Present study aimed to investigate mobility of Re&Os in W.

Modeling Method

●Density functional theory (DFT)
●VASP (Vienna ab initio Software Package)
●Projected augmented wave potential (PAW/PBE)
●$4a_0 \times 4a_0 \times 4a_0$ (128 atoms) super cell
●K-point ($3 \times 3 \times 3$)
●Cutoff energy: 350eV
●Volume relaxation

128-lattice super cell



Results

Solute atom and point defects are all attractive.

$$E_b^{sol,\alpha} = E_f^{sol} + E_f^{\alpha} - E_f^{sol,\alpha}$$

α: vacancy or SIA

$E^{sol, vacancy}$: Vacancy is located at 1st and 2nd NN position of solute atom;
$E^{sol, SIA}$: The most stable mixed-dumbbell configuration.

	1NN Vacancy (eV)	2NN Vacancy (eV)	SIA (eV)
Re	0.22	0.22	0.79
Os	0.53	0.36	1.87

Condition for RIP development
① SIA and solute atom is attractive.
② Vacancy and solute atom is attractive.
③Solute atoms must be dragged by SIA or vacancy.

Interstitial mode of solute migration is dominant.

Point defect migration energy in W-Re and W-Os alloys
(Evaluated by nudged elastic band method)

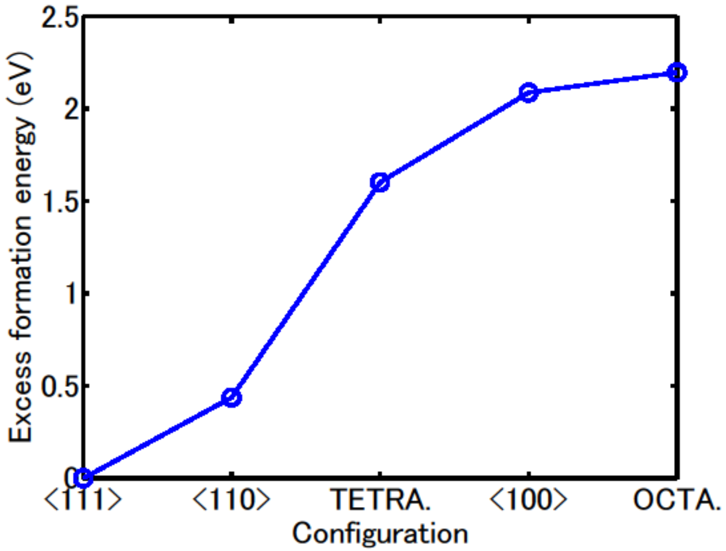
	Vacancy Mode	Interstitial Mode*
Re	1.65	0.12
Os	1.43	0.27
Self (W)	1.69	0.01

* Migration between most favorable mixed dumbbells

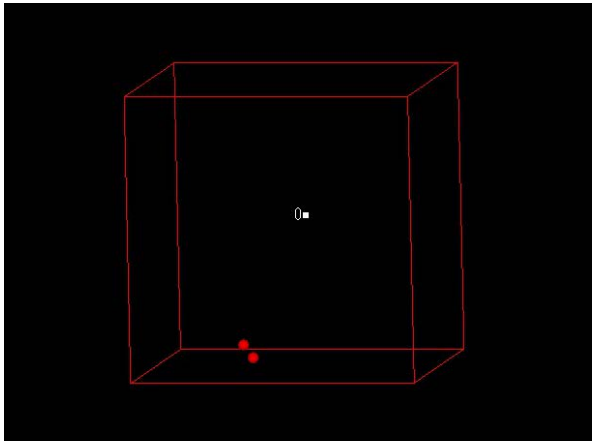
Interstitial mode of Re (Os) migration is focused.

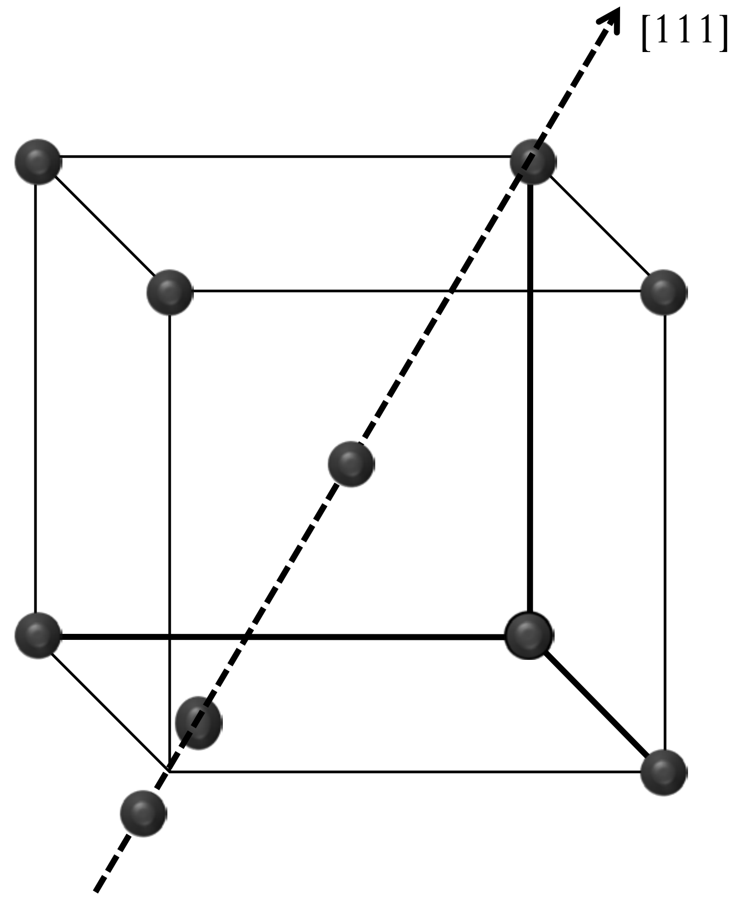
SIA has 1-dimetional motion

SIA formation energy



Self-Interstitial Atom (KMC)

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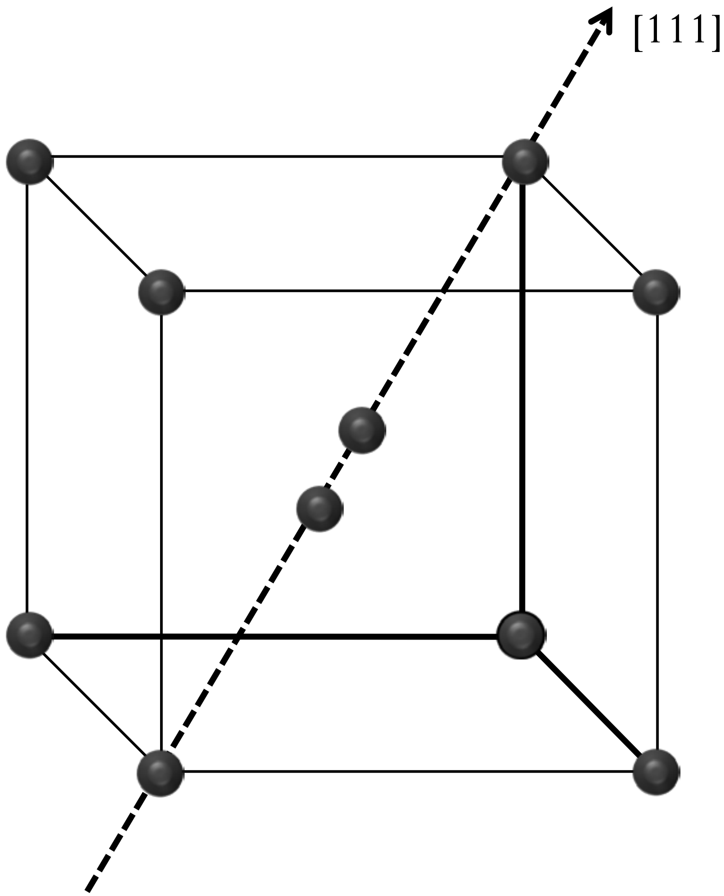
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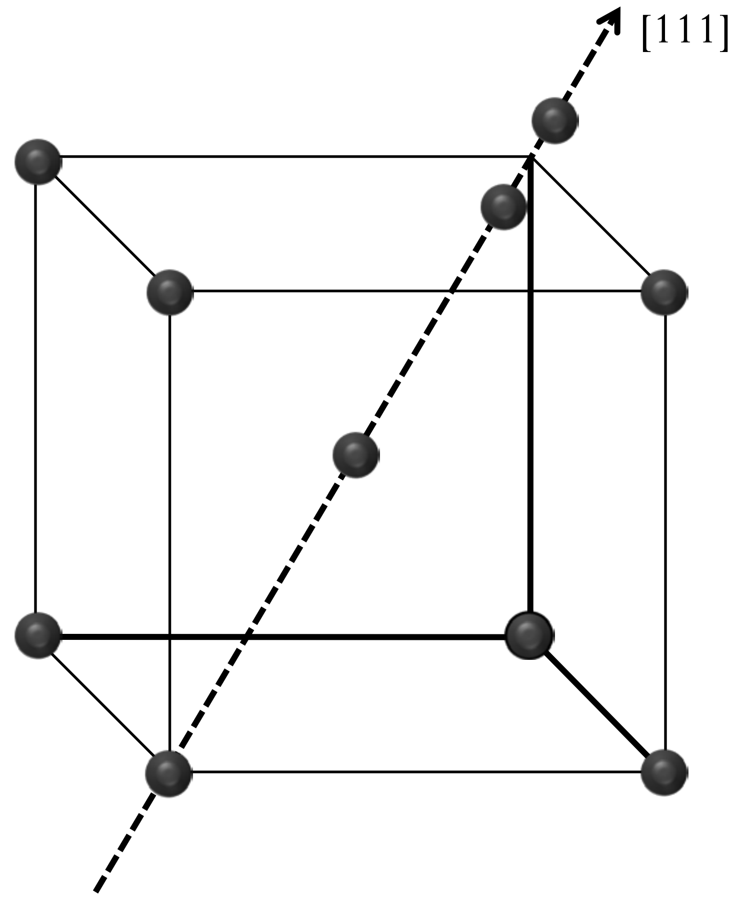
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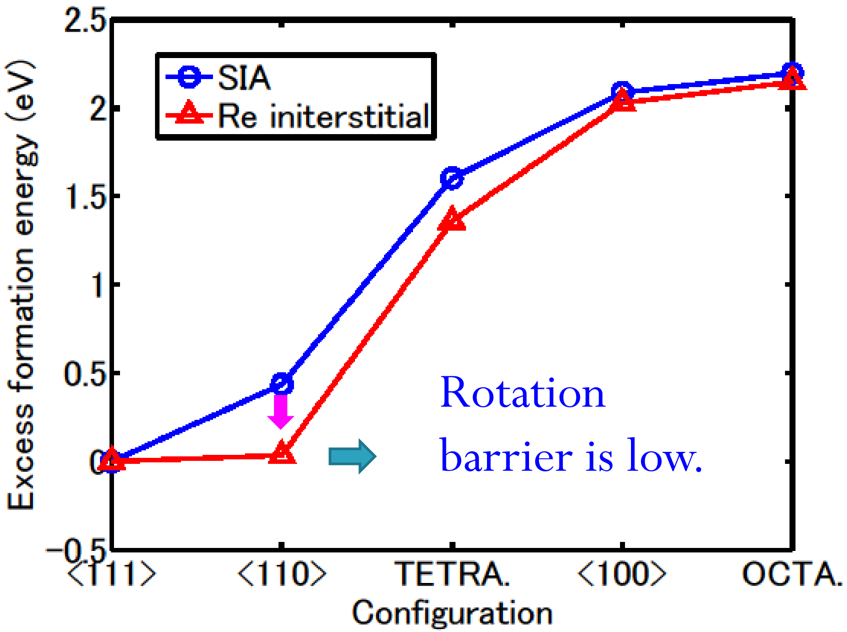
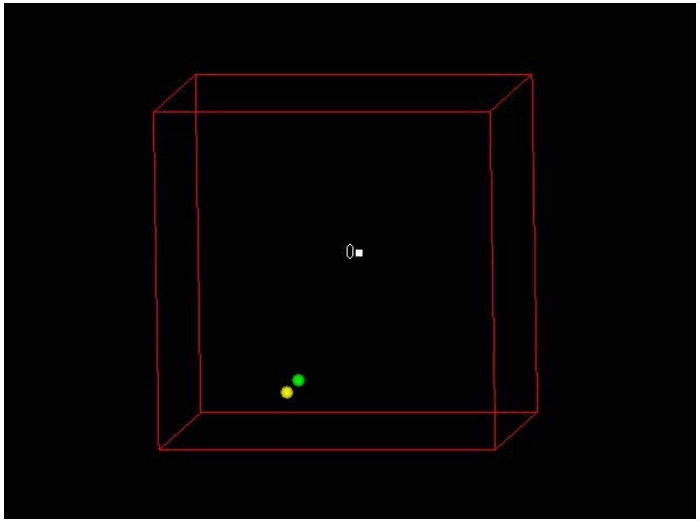
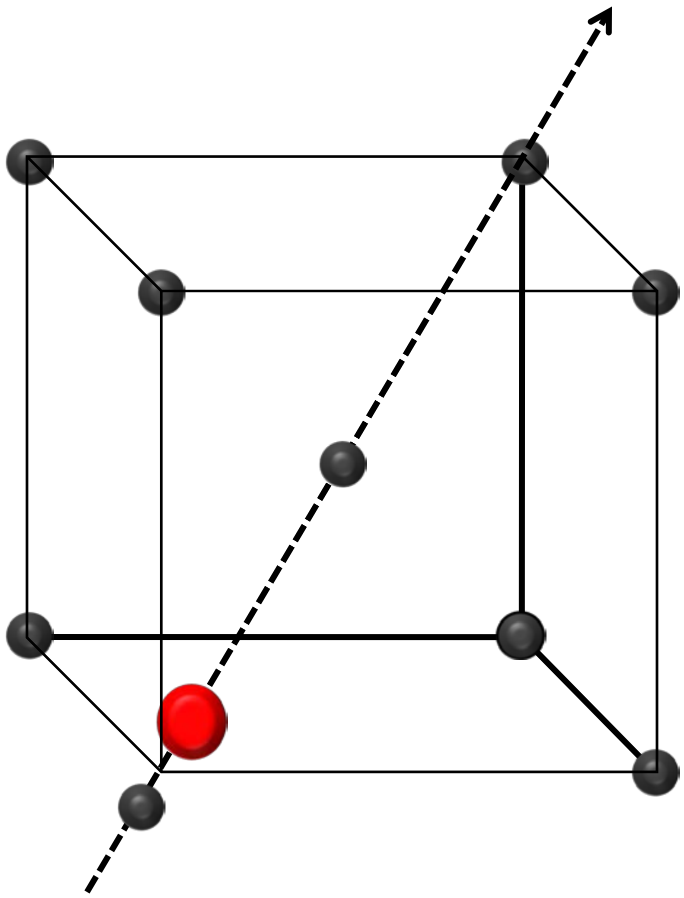
<111> W-Re mixed dumbbell has 3D motion

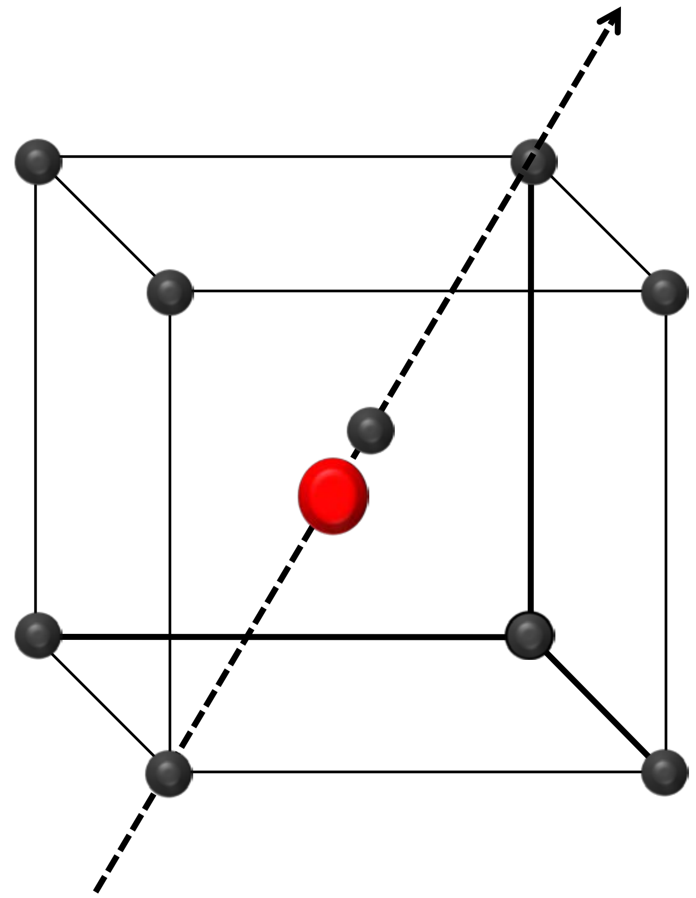
Re-interstitial formation energy

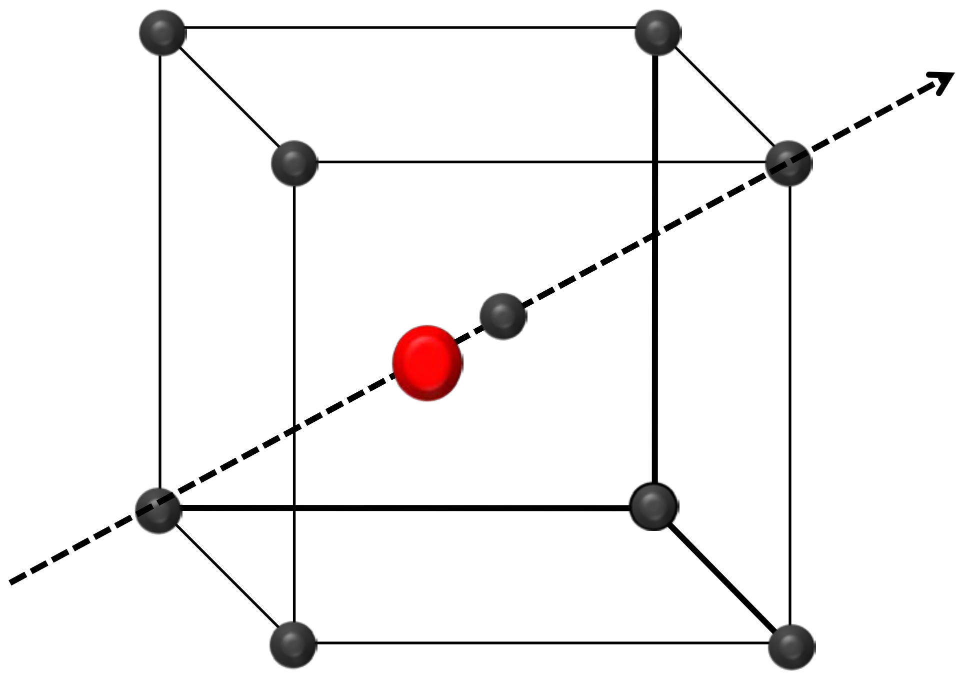


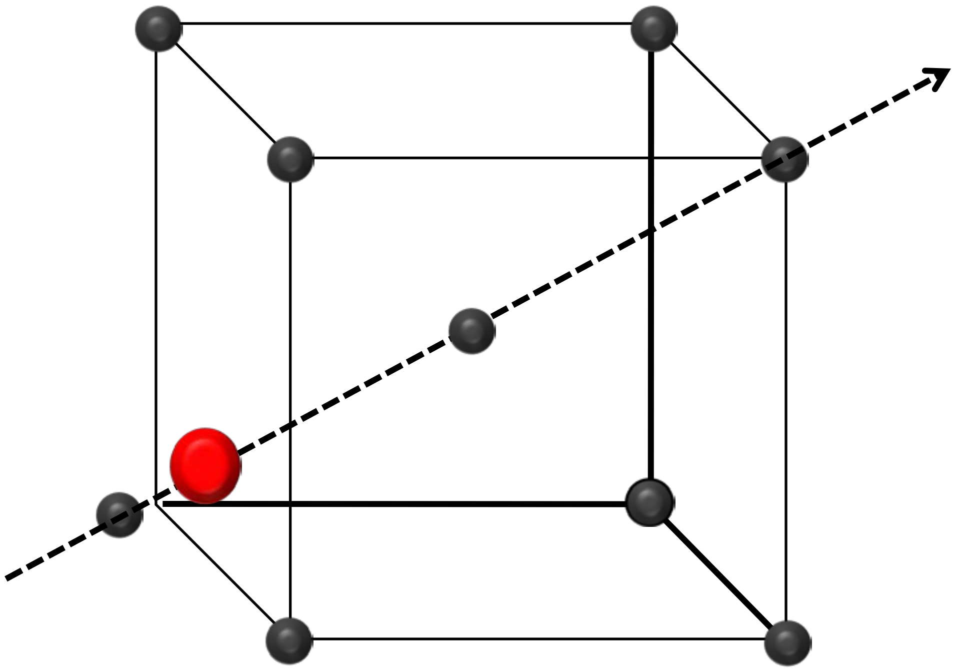
Re-Interstitial (KMC)





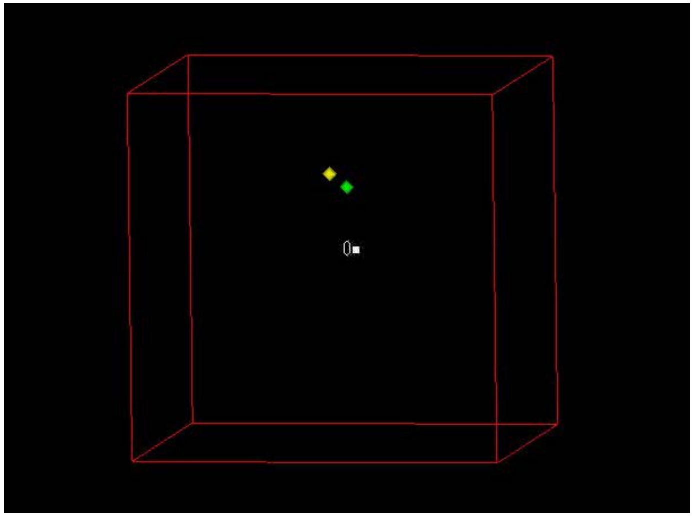




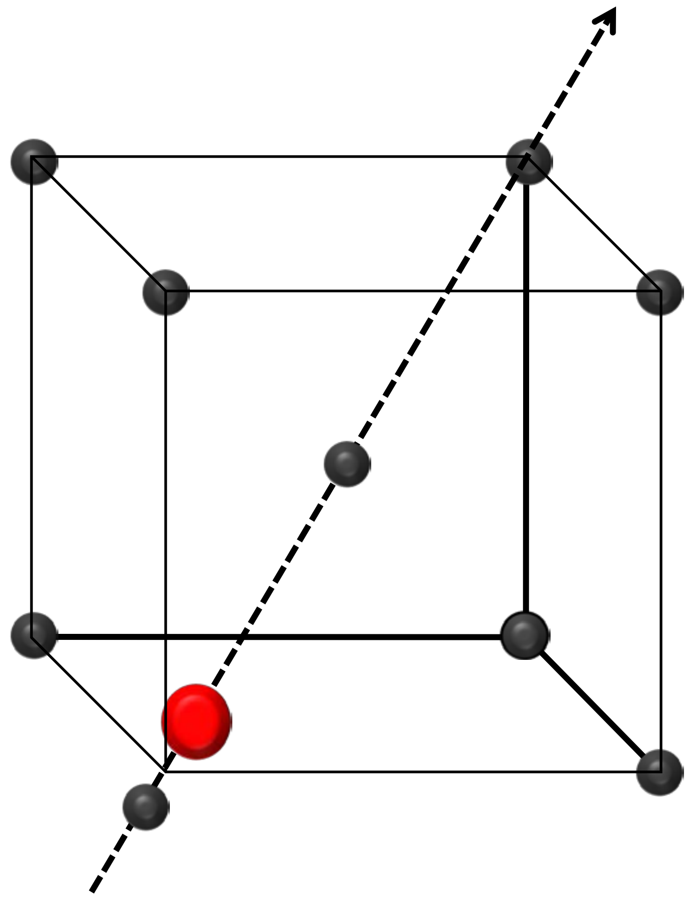


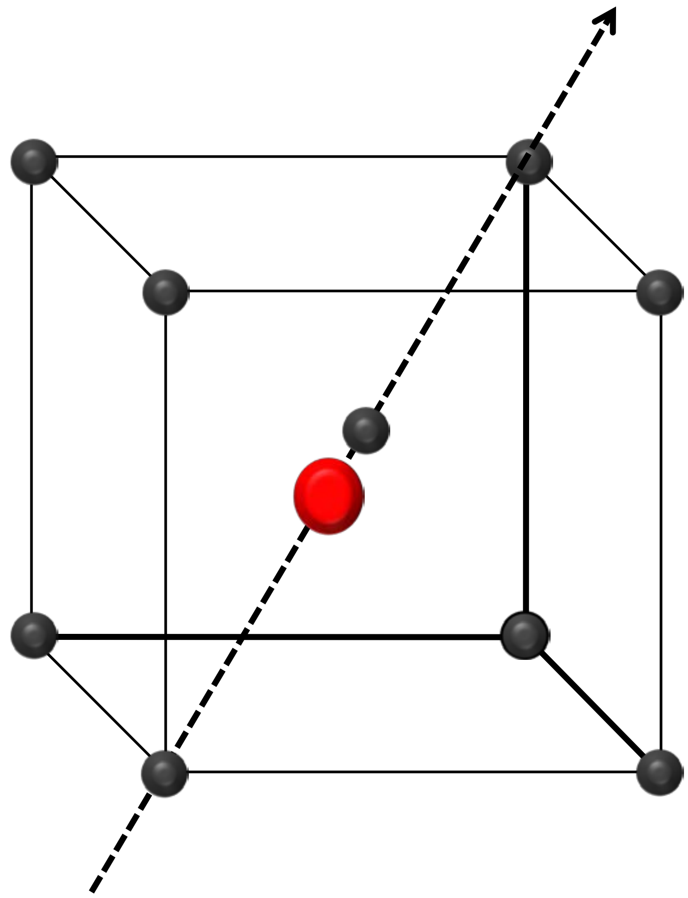
Low rotation barrier enable Re to migrate.

KMC for imaginary mixed dumbbell with rotation barrier as high as SIA



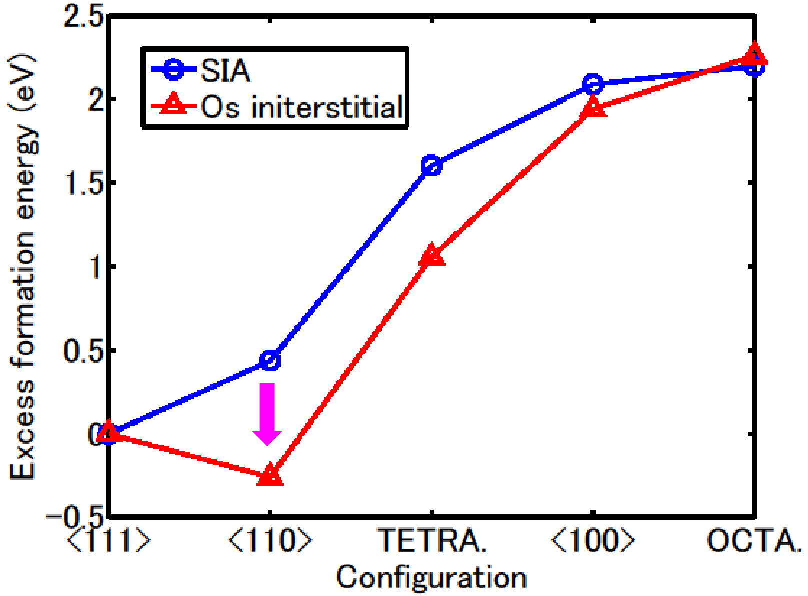
Low rotation barrier is essential to Re migration (i.e. RIP).



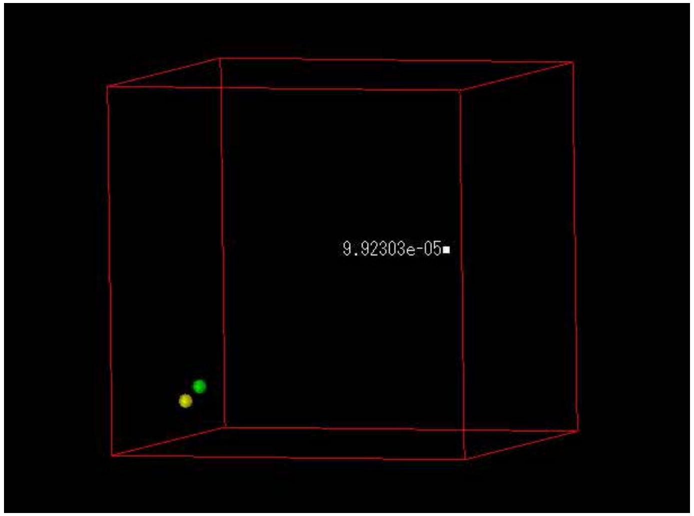


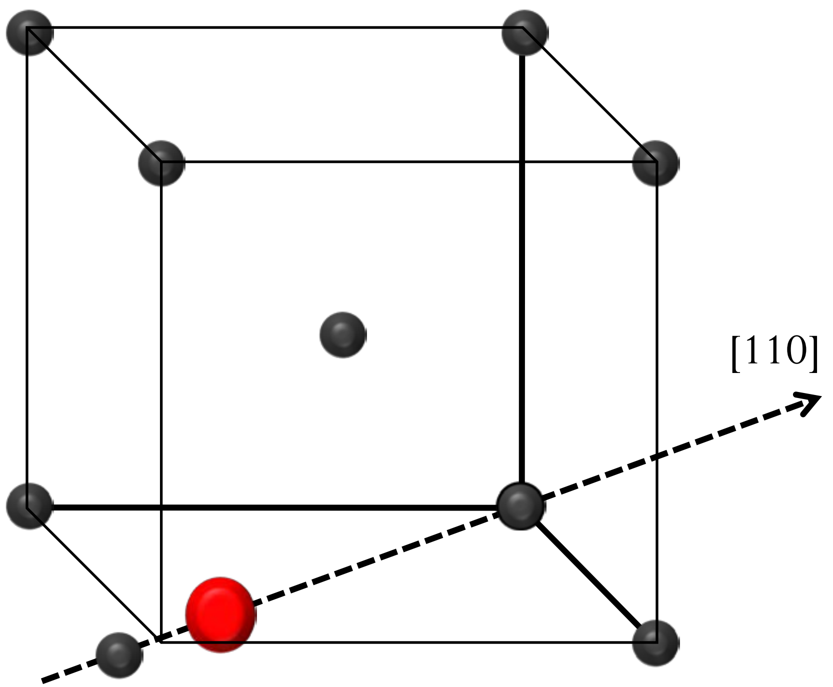
<110> W-Os mixed dumbbell has 3D motion

Os-interstitial formation energy



Os-Interstitial (KMC)

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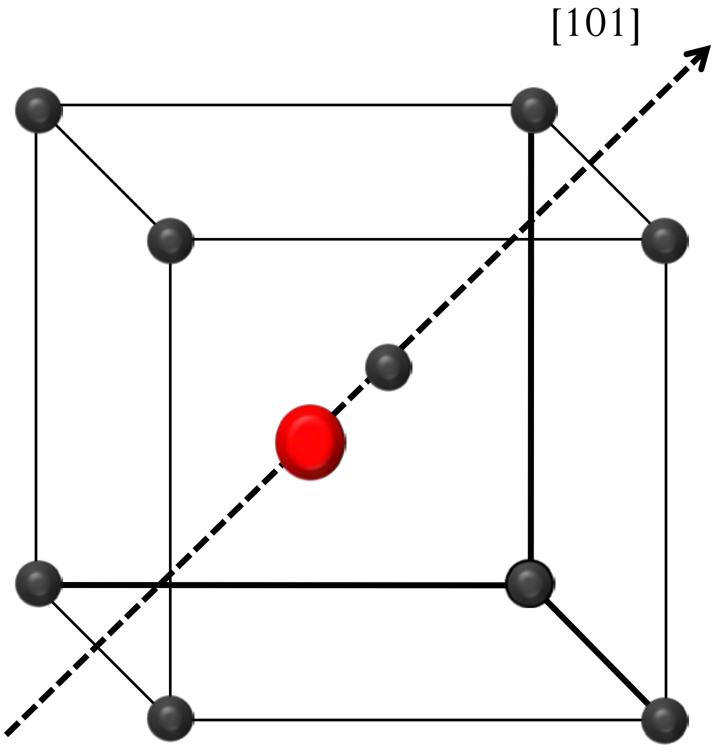
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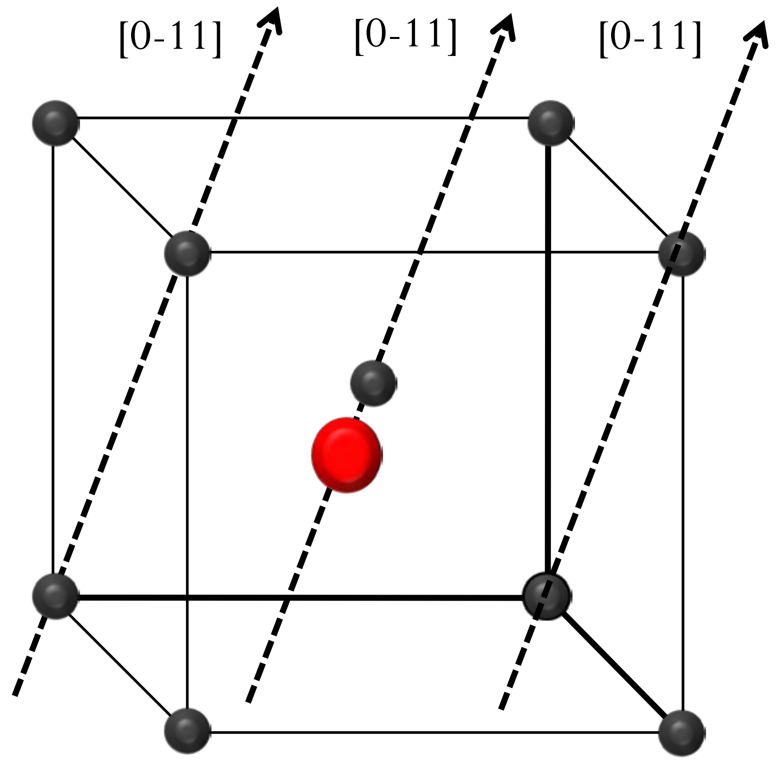
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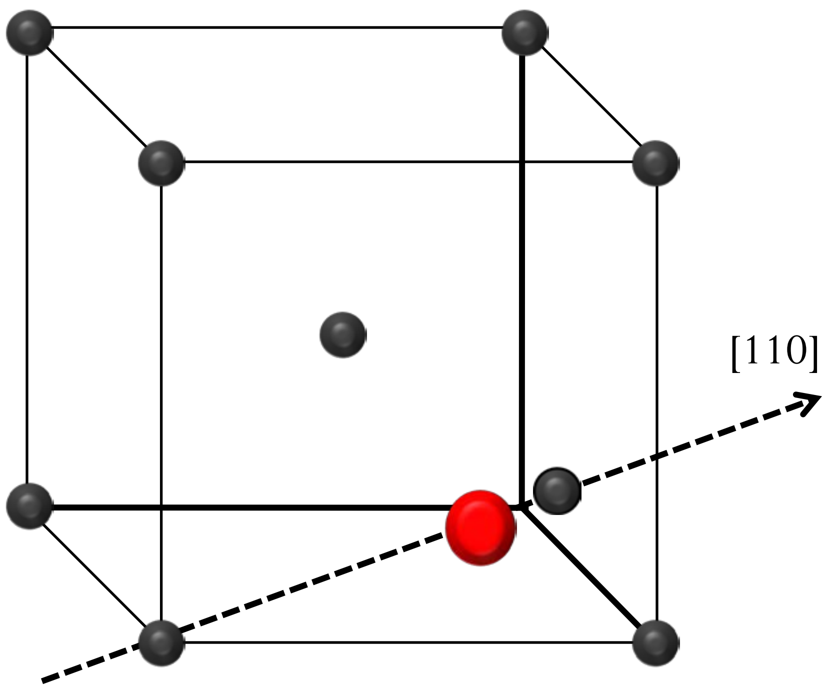
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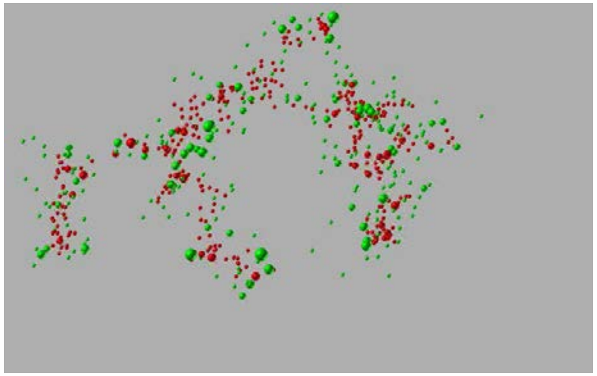
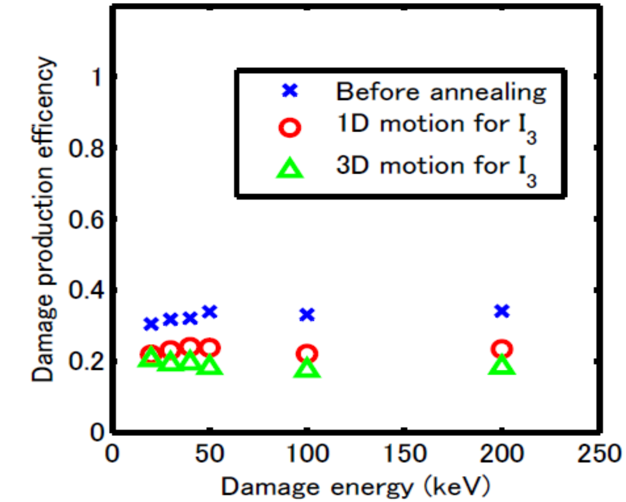
Discussion: Does 3D motion suppress radiation swelling?

KMC for cascade annealing
[T. Suzudo et al., J. Nucl. Mater. 423 (2012) 40–46.]



Surviving SIA ratio
[T. Suzudo et al., Prog. Nucl. Sci. Technol. 2, (2011) 56-63]



Defects with 3D motion promotes V-I recombination

Summary

● Re and Os in W, which are generated by transmutation, satisfy the three essential conditions for RIP.

● Re- and Os-interstitials become stable mixed dumbbell and has 3D migration mode.

● Stabilization of <110> mixed dumbbell：

1) causes solute migration, i.e., RIP?.
2) promotes V-I recombination and suppress swelling ?

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