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Grain boundary embrittlement by He segregation in bcc transition metals: Systematic study

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1. Introduction

- Neutron irradiation of ferritic/martensitic steels. at temperature less than 350℃ and He production more than 500 appm can cause a significant increase of ductile-brittle transition temperature (DBTT).
- A possible explanation, in addition to radiation hardening, may be a non-hardening embrittlement led by He segregation at GBs.
- We examined how this phenomenon can be modeled for bcc transition metals, using the combination of He-segregation rate theory and the first principles study for the GB cohesive energy ($2\gamma_{int}$).

Fig. 1 bcc transition metals in the periodic table.

2. Rate theory for He segregation kinetics

Modeling concepts are :

- A single layer of segregation sites on the GB is assumed.
- He migrates between interstitial sites in the bulk region.
- At most 1 He atom can be trapped at each segregation site.
- He can be thermally detrapped from the segregation sites.

3. First principles calculation for $2\gamma_{int}$

- $2\gamma_{int} = 2\gamma_S - \gamma_{GB}$, where γ_S is a surface energy and γ_{GB} is a GB energy.
- The loss of $2\gamma_{int}$ by solute segregation at a GB is almost linearly correlated to the increase of DBTT (**Fig. 2**); this ensures the usefulness of $2\gamma_{int}$ as a GB strength measure.
- Because the loss curve of $2\gamma_{int}$ for α-Fe is not strongly dependent on the type of GBs (**Fig. 3**)[1], we concentrated on a single particular GB type shown in **Fig. 4.** $2\gamma_{int}$ is calculated from total energy difference before and after separating the GB using the VASP code.

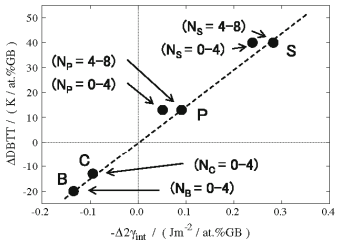

Fig. 2 Experimental shift in DBTT vs. the calculated shift in $2\gamma_{int}$ for solute atom X (X = B, C, P, or S).

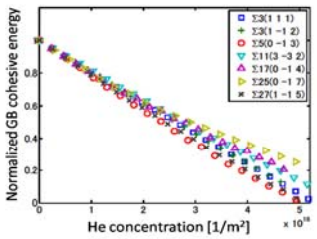

Fig. 3 $2\gamma_{int}$'s decrease caused by He segregation at various GBs: each value is normalized to $2\gamma_{int}$ for GBs without He segregation.

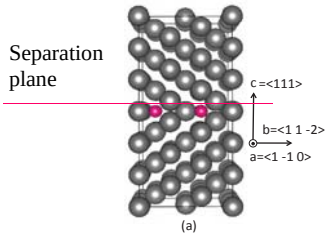

Fig. 4 The unit cell including Σ3(111) GB used in the *ab initio* study; red spheres indicate He segregation sites considered.

4. Results

4.1 He segregation kinetics:

- When the initial value of He concentration is constant over different metals, the He segregation seemed determined by He segregation energy, i.e. He binding energy to the GB (**Fig. 5**).
- E_{seg} systematically changes in the periodic table (**Fig. 6**).

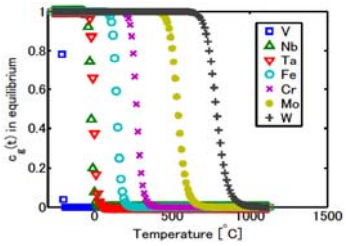

Fig. 5 He occupation ratio at segregation sites v.s. temperature..

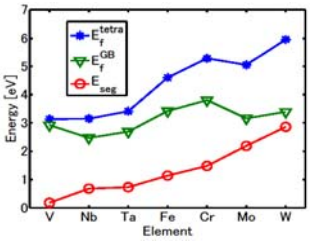

Fig. 6 He segregation energy $E_{seg} = E_{tetra} - E_f^{GB}$.

4.2 $2\gamma_{int}$ at the first wall of DEMO reactor

- Gilbert et al. [2] estimated He production rate in DEMO reactor for bcc transition metals, see **Table 1**.
- The life time estimated by them are almost inversely proportional to He production rate.

Table 1 He production rate at the first wall of DEMO and estimated lifetime, see [2]. We used data estimated for the position "A" of Fig. 2 in [2].

	He production [appm/year]	lifetime [year]
V	48	37
Nb	52	49
Ta	1.93	700+
Fe	139	6
Cr	100	8
Mo	44	46
W	4.4	700+

- We estimated $2\gamma_{int}$ at the first wall at various temperature, see **Fig.7**.
- Each graph has lower and higher shelves; The lower and higher shelves correspond to one with and without He segregation, respectively, see **Fig. 5**
- The decrease in $2\gamma_{int}$ for Ta and W at low temperatures are minimal because of their low He production rate, see **Table 1**.
- For V and Nb, the temperature range of the lower shelves are limited to the low temperature side because of the low He segregation energy, see **Fig. 6**.
- For Fe, Cr, and Mo, significant decrease in $2\gamma_{int}$ is expected at more extended temperature region.

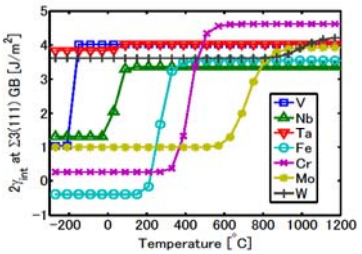

Fig. 7 $2\gamma_{int}$ at the first wall of DEMO.

5. Conclusion

- GB He embrittlement seems determined by the segregation energy and He production rate.
- The segregation energy has a systematic trend in the periodic.

References

[1] T. Suzudo, et al.: Model. Simul. Mater. Sci. Eng. 21, 085013 (2013).
[2] M. Gilbert et al.; J. Nucl. Mater. 442 S755-S760 (2013).