

## §22. Hydrogen Trapping by Vacancies in Bulk Tungsten Crystals

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Tungsten is one of the prime candidate plasma-facing materials at ITER, which would be exposed to high fluence of hydrogen. Some experimental studies showed that the amount of retained deuterium in deuterium-implanted tungsten was of the same order of magnitude as in graphite. Trapping sites in tungsten are however not fully identified yet.

Previously, we investigated the binding energies between hydrogen atoms and mono-vacancies in tungsten by means of the first principle molecular dynamics code, VASP<sup>1)</sup>. The calculated binding energies were consistent with values inferred from thermal desorption spectra of the deuterium-implanted tungsten<sup>2)</sup>.

Thermodynamic properties of a bulk tungsten crystal (bcc) containing the mono-vacancies and hydrogen atoms were studied by taking account of the calculated binding energies. At thermal-equilibrium, average numbers for trapped hydrogen atoms at the single mono-vacancy and the vacancy concentration were evaluated as functions of local hydrogen concentrations for different temperatures.

Fig. 1 illustrates the bulk tungsten crystal containing  $N_0$  tungsten atoms,  $N_H$  hydrogen atoms, and  $n$  mono-vacancies.  $rn$  hydrogen atoms are trapped among  $6n$  octahedral sites of the mono-vacancies, and residual  $N_H - rn$  hydrogen atoms are distributed over  $6N_0$  interstitial (tetrahedral) sites. Partition functions  $Z$  of this system at a given temperature  $T$  are approximated by,

$$Z = Z_M \times Z_1,$$

$$Z_M = \frac{(N_0 + n)!}{N_0! n!} \exp(-nf_i/kT), \quad (1)$$

$$Z_1 = \frac{(6N_0)!}{(N_H - rn)!(6N_0 - N_H + rn)!} \exp[-(N_H - rn)f_s/kT] \times \frac{(6n)!}{(rn)!(6n - rn)!} \exp(-nf'_s/kT),$$

where  $f_i$ ,  $f_s$  and  $f'_s$  are the formation energy of the bare mono-vacancy, the solution energies of the interstitial hydrogen atom and the hydrogen atom trapped at the mono-vacancy, respectively. Those energies were obtained from the present first principle calculations. The average number of hydrogen atoms trapped by one mono-vacancy, i.e.  $r$ , is obtained under the condition that the free energy of

the partition function, eq. (1), has the minimum value.

Fig. 2 shows variation of the mono-vacancy concentration in the bulk tungsten crystal as functions of the hydrogen concentration. For low hydrogen concentration, the vacancy concentration at a given temperature has a certain value determined by the formation energy of the bare mono-vacancy. Above some threshold values of the hydrogen concentration, the vacancy concentration shows rapid increase. It turns out that the rapid increase of the vacancy concentration is associated with increase in the average number of the hydrogen atoms trapped by the vacancy.

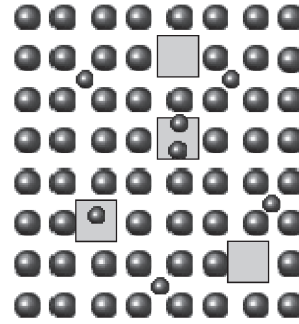


Fig. 1: Illustration of the bulk tungsten (larger balls) crystal containing mono-vacancies (squares) and hydrogen atoms (smaller balls).

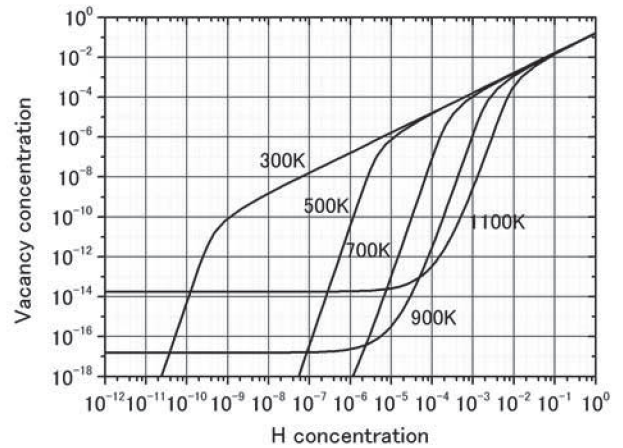


Fig.2: Vacancy concentration at thermal equilibrium as functions of hydrogen concentration at five temperatures for 300-1100K.

- 1) Kresse, G. and Furthmüller, J.: Phys. Rev. B 54 (1996) 11169.
- 2) Garcia-Rosales, C. et al.: J. Nucl. Mater. 233-237 (1996) 803.