

## §9. Hydrogen Retention in Bulk Tungsten Crystals under Hydrogen-rich Condition

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Tungsten is one of the prime candidate plasma-facing materials at ITER, which would be exposed to high fluence and flux 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. Recently, fine grain tungsten specimens showed suppression of hydrogen blistering, which suggest that grain boundaries of tungsten may serve as bypasses for hydrogen evacuation. Micro structures inside grains are responsible for hydrogen retention. Theoretical models to describe development of the micro structures under hydrogen-rich conditions are highly desirable.

Previously, we investigated 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 specimens. It may suggest that vacancies inside the grains are responsible for the hydrogen retention of tungsten.

Thermodynamic properties of a bulk tungsten crystal (bcc) containing the mono-vacancies and hydrogen atoms were studied using the calculated binding energies. According to partition functions of Boltzmann statistics, variation of thermal-equilibrium values of the mono-vacancy concentration along the hydrogen concentration showed a steep raise at a certain value of the hydrogen concentration determined by a given temperature. Higher temperatures generally give larger fractions of interstitial (solution) hydrogen atoms. The steep increase of the mono-vacancy concentration is associated with increase of fraction of trapped (precipitate) hydrogen atoms at the mono-vacancy<sup>1)</sup>.

Vacancy cluster formation (coaggregation) in the crystals is also an issue of study. From present studies, it has turned out that the first principle (density functional theory) calculations gave correct mono-vacancy formation energies, provided that corrections in exchange-correlation energies (xc-energies) were properly taken into account. VASP code with PBE-type xc-energies gives the mono-vacancy

formation energy of 3.2 eV (for a super cell of 128 atoms), cf. 3.1 – 3.7 eV values in Landolt-Börnstein<sup>2)</sup>. Electron density distribution has a hole at the vacancy. The electron density varies abruptly across edges of the hole. The PBE-type xc-energies may give inaccurate results for electron energies with such abrupt variation of electron densities. Errors in the PBE-type xc-energies are estimated for tungsten, and about 0.4 eV should be added to calculated values of the mono-vacancy formation energy.

Several configurations are possible to introduce another vacancy nearest neighbor to the principal vacancy in the bcc crystal (see Fig. 1). Di-vacancy binding energies: energy lowering by formation of single di-vacancy than formation of two mono-vacancies apart from each other, have been studied previously by utilizing some empirical models for inter-atomic interaction potentials. The second nearest neighbor configuration ([100] direction to the principle vacancy, 2NN in Fig. 1) has the largest binding energy of 0.78 eV in the previous studies<sup>3)</sup>. The first principle calculations of the di-vacancy binding energies are ongoing.

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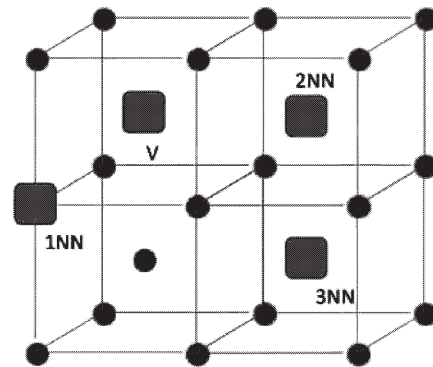


Fig. 1: Illustration of nearest neighbor configurations of di-vacancy in the bcc crystal. V stands for the principle vacancy, 1NN the first nearest neighbor [111], 2NN the second nearest neighbor [100], and 3NN the third nearest neighbor [110] sites, respectively.

- 1) Kato, D., Iwakiri, H. and Morishita, K.: Proc. 14<sup>th</sup> Int. Congress Plasma Phys., Fukuoka, Japan, Sept. 2008, JPFR Ser. in press.
- 2) Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology 25, *Atomic Defects in Metals* (ed. Ullmaier, H.).
- 3) Johnson, R.A.: Phys. Rev. B 27(4) (1983) 2014-2018.