§19. First-principles Study of Vacancy Migration in Tungsten

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In ITER, pure tungsten and tungsten alloys are considered to be one of the most promising candidates for divertor plates. Thermal vacancies generate in tungsten material when tungsten material is exposed to high temperatures. The diffusion and aggregation of vacancies embrittle tungsten material. In addition, it is also considered that the diffusion of vacancies in tungsten material is effective against the formation of helium bubble[1] in tungsten material and tungsten fuzzy nano-structure[2]. These diameters are in nanometer-scale. This fuzzy structure causes the embrittlement of the divertor material. And the embrittlement causes the impurity release into vessel. However, from the viewpoint of device application as nano-materials, fuzzy structure can be used as a nano-catalyst and a stray light measures material because the tungsten material with fuzzy structure has a large surface area and the property that the reflectance is almost zero. In the above background, it is necessary to reveal the mechanism of the tungsten nano-structure formation. The key point of bubble structure creation is the trapping of helium atoms into thermal vacancies in the tungsten lattice structure. It is pointed out that the bubble has influenced the formation of fuzzy structure.

We have evaluated the migration energies of mono-vacancy and di-vacancy and the binging energy of di-vacancy in tungsten material by the first-principles calculation based on the DFT[3,4]. The DFT is a powerful tool to estimate the energies of materials in the atomic scale. For example, the calculation with the DFT by Takayama *et al.*[5] showed that helium atoms aggregate in mono-vacancy. The migration energy and reaction path were estimated with a combination of the DFT and the nudged elastic band (NEB) method[6].

DFT calculations are performed by the Open source package for Material eXplorer (OpenMX)[7]. Total energies are calculated for a bcc supercell composed of 128 tungsten atoms ($4\times4\times4$).

Migration of a single vacancy in a bcc lattice has only two possible migration pathways: along the [001] and [111] direction. The migration energies of mono-vacancy in the [111] and [001] direction is 1.78 and 5.54 eV, respectively. It is understood that a mono-vacancy diffuses in the [111] direction easily rather than in the [001] direction.

Figure 1 shows the initial and final paths of the NEB calculations of di-vacancy. The final paths of the NEB show that the tungsten atom moves in the [111] direction even if the moving distance is long. A tungsten atom moves in the [001] direction only when it cannot move in the [111] direction.

Table I shows the migration energies of the paths of Fig. 1. The migration energies of path (a), (b), and (c) are almost the same value of the mono-vacancy. The migration energy of path (d) is the same value as the migration energy of the [111] and [001] directions of the mono-vacancy. In other words, migration of di-vacancy is approximately the same as the migration of mono-vacancy.

The di-vacancy binding energies for different configurations were represented in Table I. The interactions between two vacancies in tungsten material are unexpectedly repulsive from the second to fifth nearest-neighbor and that the second nearest-neighbor di-vacancy is the most repulsive. In tungsten material, di-vacancy is less stable than mono-vacancy. Hence, vacancies in tungsten material are difficult to aggregate.

We calculated the binding and migration energies of vacancies. By the comparison of these energies between helium atoms and vacancies, we can determine which the self-aggregation of the helium and aggregation of vacancy is dominant process in the formation of the helium bubble.

Table I Migration energies of di-vacancy.

	Path (a)	Path (b)	Path (c)	Path (d)
Migration energy [eV]	1.75	1.73	1.65	5.30

Table II Binding energies of di-vacancy. The interactions between two vacancies in tungsten material are repulsive from the second (2NN) to fifth nearest-neighbor (5NN).

	1NN	2NN	3NN	4NN	5NN
Binding energy [eV]	0.03	-0.28	-0.01	-0.04	-0.08

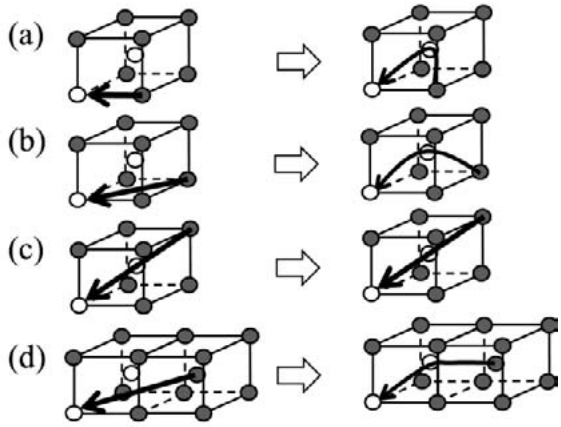

Fig. 1. Migration paths of di-vacancy of NEB calculations. Left and right side are the initial and final paths of NEB calculations, respectively. Open circles and grey circles indicate vacancies and tungsten atoms, respectively.

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