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First principle calculations of energy of agglomerated helium in the period 6 elements

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ABSTRACT

Difference of helium (He) agglomeration energies between period 6 elements, tantalum (Ta), tungsten (W), iridium (Ir) and gold (Au), is illustrated by using first principles calculations based on density functional theory (DFT). It is found that He in W and Ir can agglomerate more easily than Ta and Au. We investigate a relationship between the He agglomeration tendency and the growth of nanostructure by He plasma irradiation. Thus, the four metals are exposed to He plasma irradiation. Each metal has different structures after the He plasma exposure. Surface nanostructures of W and Ir are fuzzy fiber-like while these structures are not observed in Ta and Au. In the meantime, W and Ir have a tendency to agglomerate He atoms at a vacancy or interstitial sites easily. This correlation suggests that the He agglomeration may play a role for understanding the fuzz formation mechanism.

1. Introduction

Tungsten (W) has high melting point, high thermal conductivity and low sputtering yield [1]. It is an important plasma facing material due to its properties. Because helium (He) atoms are produced by Deuterium-Tritium (D-T) fusion reaction, interaction of He with W was widely studied [2–5]. After He plasma exposure with low incident energy, the formation of fiber-like nanostructures at W surface, known as fuzz structure, were observed. These structures can be a safety concern because of its fragility and its potential to cause self-arcing. It is important to understand their formation mechanism from the aspect of reactor maintenance management. However, it has not been understood well.

It is presumed that fuzz formation process differs from deposition process and sputtering process from experimental research. Before growth of fiber-like nanostructures, hole formations or loop-like structures appear [4]. He bubbles were observed on fiber-like nanostructures from transmission electron microscope (TEM) images [5]. In addition to W, it has been reported that the nanostructures of several metals are also induced by the He plasma irradiation. The nanostructures of titanium (Ti) [6], vanadium (V) [7], iron (Fe) [6], nikkel (Ni) [6], niobium (Nb) [8], molybdenum (Mo) [9], tantalum (Ta) [10] and rhenium (*Re*) [9] has been found. We believe that the comparison between metals in nanostructure formation provides key information for understanding the formation mechanisms. One of the key information is the evaluation of the binding energy of He atoms in metals by using first principles calculations based on the density functional theory (DFT) [11]. Recently, we have compared He plasma induced nanostructures and the He agglomeration tendency between group 5 elements (Nb and Ta) and group 6 elements (Mo and W) using the DFT calculations [12]. Consequently, we have found similarities between the same group elements for the experimentally observed nanostructures. Moreover, the similarity between the same group elements was confirmed in microscopic He properties, i.e., He agglomeration tendencies in a vacancy and an interstitial site, simulated by DFT.

In the present work, we investigated a difference of He agglomeration energies for metals with agglomerated He atoms between period 6 elements (Ta, W, Iridium (Ir) and gold (Au)) by using the DFT calculations to investigate further on the relationship between the shape of He induced surface structures and the atomic level properties due to He agglomeration,

2. Simulation method

We employed first principles calculations based on DFT to investigate differences in the He agglomeration characteristics. The calculations were done by the OpenMX code package [13]. Norm-conserving pseudopotentials [14–18] and pseudo-atomic localized basis

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Table 1
Solution energies of He in tetrahedral site and octahedral site and the calculated vacancy formation energies in Ta, W, Ir and Au.

	Ta	W	Ir	Au
$E_{\mathrm{sol,oct}}$ (eV)	4.15 [12], 3.42 [22]	6.44 [12], 6.38 [23]	3.84	3.17
$E_{\mathrm{sol,tet}}$ (eV)	3.81 [12], 3.16 [22]	6.19 [12], 6.16 [23]	4.24	3.28
E_{vac}(eV)	3.08	3.49, 3.11–3.46 [23], 3.6 [25], 4.0 [26]	1.88	0.56

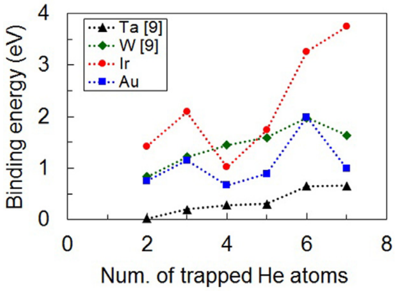

Fig. 1. The calculated binding energies at an interstitial site with n agglomerated He atoms in Ta, W, Ir and Au.

Table 2
The calculated binding energies (eV) at interstitial sites with n agglomerated He atoms in Ta, W, Ir and Au.

He	Ta [12]	W [12]	Ir	Au
2	0.03	0.83	1.43	0.75
3	0.20	1.22	2.10	1.15
4	0.29	1.44	1.02	0.67
5	0.31	1.60	1.74	0.89
6	0.65	1.97	3.26	1.99
7	0.66	1.64	3.75	0.99

functions [19,20] were employed. The generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) functional [21] was used for the exchanged-correlation potential.

Total energies were calculated for body-centered cubic (bcc) (Ta, W) supercells composed of 128 or 127 metal atoms (4 × 4 × 4 unit cells) and face-centered cubic (fcc) Ir or Au supercells composed of 108 or 107 metal atoms (3 × 3 × 3 unit cells) with n He, where n is a number of He atoms to be agglomerated at one interstitial site. In the present calculation, the structure relaxation was not performed, thus the condition was the fixed simulation cell. From the pre-calculations with the unit cell system, the lattice constants are obtained to be 3.317 Å for Ta, 3.186 Å for W, 3.877 Å for Ir and 4.169 Å for Au.

3. Result and discussion

3.1. He binding energies at interstitial sites

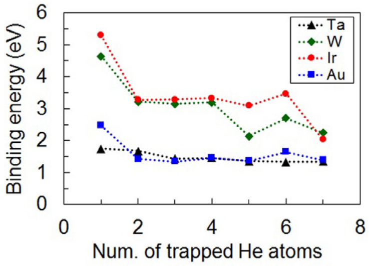

Fig. 3. The calculated binding energies at a vacancy with n agglomerated He atoms in Ta, W, Ir and Au.

Table 3
The calculated binding energies (eV) at a vacancy with n agglomerated He atoms in Ta, W, Ir and Au.

He	Ta	W	Ir	Au
1	1.75	4.65	5.30	2.48
2	1.68	3.21	3.28	1.43
3	1.44	3.15	3.29	1.35
4	1.46	3.19	3.33	1.46
5	1.36	2.14	3.10	1.37
6	1.33	2.70	3.47	1.64
7	1.35	2.25	2.03	1.39

We calculated the binding energy at interstitial sites E_{int} (n) to investigate differences in the He agglomeration characteristics. It is given by

$$E_{\mathrm{int}}\ (n) = -E\ (\mathrm{He}_n\ \mathrm{Me}_N) - E\ (\mathrm{Me}_N) + E(\mathrm{He}_{n-1}\ \mathrm{Me}_N) + E(\mathrm{He}_1\mathrm{Me}_N), \tag{1}$$

where $E(\mathrm{He}_n\ \mathrm{Me}_N)$ is the total energy of the metal (Me) composed of N atoms with n agglomerated He atoms. Because there are two interstitial sites in bcc and fcc structures, we investigated the most stable site for E $(\mathrm{He}_1\ \mathrm{Me}_N)$. According to previous results [6,16,17], the tetrahedral site is more stable as a He trap site than the octahedral site in Ta and W, which have a bcc structure. Table 1 shows solution energies of He in tetrahedral site and octahedral site. It is given by

$$E_{\mathrm{sol}} = E(\mathrm{He}_1\mathrm{Me}_N) - E\ (\mathrm{Me}_N) - E\ (\mathrm{He}_{\mathrm{isolated}}), \tag{2}$$

where $E(\mathrm{He}_{\mathrm{isolated}})$ is the energy of the isolated He atom. The octahedral site is energetically more stable than the tetrahedral site in Ir and Au, which have the fcc structure. Therefore, we positioned He on a tetrahedral site in the bcc structure cases and an octahedral site in the fcc structure cases when we calculated $E(\mathrm{He}_1\ \mathrm{Me}_N)$.

Fig. 1 and Table 2 show the binding energies at interstitial sites in Ta, W, Ir and Au. The binding energies of Ta are smaller than those of W, Ir and Au. The results in Ta and W agree with the results of You et al. [11] and Huang et al. [24]. As seen in Fig. 1, there are similarities in the binding energy tendency between Ta and W, and between Ir and Au. The tendency of binding energies is related to crystal structure types. For example, both Ta and W show increasing binding energies up to n = 6 He cluster. Then, binding energy for the 7th He atom becomes lower or similar with the 6th He atom. We speculate that this tendency is caused by He cluster shape in lattice. Our results show same $\mathrm{He_n}$ cluster shape for n = 2–6 in the bcc or fcc structure. Fig. 2 shows the differences of He_7 cluster shape in each metal. Cluster shape becomes

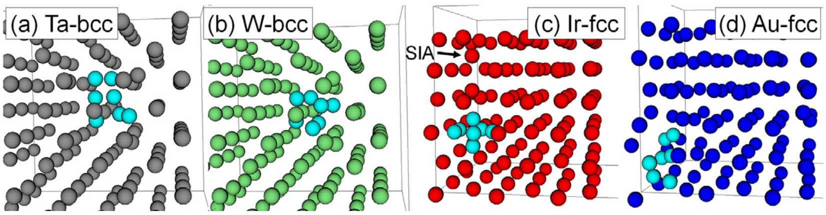

Fig. 2. The structure of He_7 cluster in (a) Ta, (b) W, (c) Ir and (d) Au. The grey, green, red, blue and light blue spheres indicate Ta, W, Ir, Au and He. He atoms aggregated at interstitial sites in Ta, W, Au while He atoms aggregated at a vacancy and a SIA was emitted from He_7 cluster in Ir.

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