

Investigation of interaction of He and D in FeBSi alloy

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Abstract

He and H can be produced by nuclear reaction. In addition, energetic particles of He and T and D, which are isotopes of H, in the plasma of fusion reactor induce the damage in the surface of materials, such as erosion, sputtering and blistering. To investigate the interaction of He and D, amorphous and crystalline FeBSi alloys were irradiated by He or D₂ or He+D₂ ions with 5 keV. The results of thermal desorption indicated that more He atoms were trapped in both amorphous and crystalline alloy irradiated by He ions than D atoms in those alloy irradiated by D₂ ions. Although He and D atoms were trapped FeBSi alloy irradiated by He+D₂ ions, desorption peaks of D₂ and He were separate. Absorption of D in amorphous alloy was influenced by the presence of He, however, absorption of He was independent of D₂ irradiation in both alloys.

Keywords: amorphous alloys, defects in solids, damage, helium, deuterium

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1. Introduction

Interest in the behavior of He, H and its isotopes in solids has increased with advances in fusion reactor technology. He and H are generated in materials by the nuclear reaction of (n, α) and (n, p) , which increases with increasing neutron energy. In addition, He and D and T, which are isotopes of H, are also introduced directly into plasma-facing materials (PFMs) by the plasma in fusion reactors. He atoms are insoluble in most metals and alloys, and the presence of He atoms in metals may have a great impact on the microstructure. He, which has a strong interaction with vacancies [1, 2], forms a high density of helium bubbles and induces void swelling. In addition, He atoms also promote the nucleation of dislocation loops [3, 4]. It is reported that H atoms prevent the reaction of vacancies and dislocations with free interstitials, as a result increasing nucleation dislocation loops [5].

In most of candidate first wall and divertor materials for fusion system, such as austenitic steels, ferritic steels and copper alloys, He and H are produced simultaneously by not only fission neutrons but also fusion neutrons. Consequently, it is impossible to know how He and H influences nucleation and growth of dislocations and voids, and whether there is an interaction between He and H or not during microstructural evolution. To separate the intrinsic effects of He or H and the synergetic effects of He and H on microstructural evolution, B addition and isotopic tailing methods are used to investigate the He effect on void swelling [6-11]. These experimental results show that both He and H enhanced the void swelling, and He effect on void swelling was more prominent. However, it is difficult to distinguish separate effects and synergetic effects of He and H in materials where

both He and H are produced during irradiation. Recently, interaction of He and H in Fe was investigated by Geng *et al.* using *ab initio* density functional theory calculations [12]. It is attraction interaction between He and H in bulk, and repulsion interaction in grain boundary in bcc Fe. In order to clear the interaction between He and H, amorphous and crystalline FeBSi alloys were irradiated by He or D₂ or He+D₂ ions, and then, desorption of He and D₂ was analyzed by annealing the irradiation samples. The reason for substitution of H by D, isotope of H, is that the sensitivity of D is higher than H.

2. Experimental procedure

The amorphous alloy Fe₇₉B₁₆Si₅ (Metglas 2605S-3) was obtained in the form of sheets 25 μm thick, which was prepared by contact with a simple copper roller in an atmosphere of argon. The crystallization temperature (T_c) of the as-quenched Fe₇₉B₁₆Si₅ alloy was ~ 788 K. Crystalline FeBSi alloy specimens were prepared in a vacuum furnace by rapidly heating amorphous ribbons to 923 K for 0.5 hours. The amorphous and crystalline samples were irradiated by single irradiation with 5 keV He⁺ ions or 5 keV D₂⁺ ions, and double irradiations with 5 keV He⁺ + 5keV D₂⁺ ions or 5 keV D₂⁺ + 5keV He⁺ ions using an Omegatron gun, in which mono-energetic He⁺ and D₂⁺ ions were collimated and mass-analyzed. The irradiation dose for each ions was 1.0×10^{20} ions/m². The displacement damage region was 50 nm from the incident surface, and the peak of displacement damage was 15 nm according to the calculations using TRIM code [13], where the threshold displacement energy in FeBSi amorphous alloy was assumed to be 40 eV. Afterwards, thermal desorption spectroscopy (TDS) analysis was performed by heating the samples to

1253 K using infrared irradiation. The ramping rate of the temperature was fixed at 1 K/s. During heating, The gas releases were monitored by a quadruple mass analyzer. The quadruple mass analyzer used in the present study was not high resolution, therefore, the small mass difference between D₂ and He (D₂: m=4.0282 amu and ⁴He: m=4.0026 amu) could not distinguished by our QMS. In order to distinguish the gas of D₂ and He, the gas with atomic mass of 3, which comes from gas of HD, was monitored. It is possible to form HD during D release, but it is impossible to form HD during He release.

3. Results and discussion

Fig. 1 shows D₂ thermal desorption from amorphous (a) and crystalline FeBSi (b) after 5 keV D₂ irradiation to 1.0×10^{20} D₂/m². In both alloys, only one peak appeared clearly at temperature of about 340 K, which was thought that D₂ was trapped by the surface defects produced by the irradiation [14]. In addition, the background of D₂ thermal desorption in amorphous alloy was higher than that in crystalline alloy at the temperature below 650 K. Desorption of mass 3 in the same alloys is also shown in Fig. 1. The sharp peaks of mass 3 overlapped those of mass 4. Desorption of mass 4 increased desorption of mass 3 because gas of HD is related to gas of D. The broad peak of mass 3, on the other hands, was not related to desorption of D₂. It comes from desorption of H absorbed by surroundings.

Fig. 2 shows He thermal desorption from amorphous (a) and crystalline FeBSi (b) after 5 keV He irradiation to 1.0×10^{20} He/m². Compared with D₂ irradiation, He thermal desorption peaks, which were higher than D₂ thermal desorption peak, appeared at high temperatures besides the peak at low temperature of about 330 K. The peak at 330 K arose from He that was trapped by the surface defects similar to D₂ thermal desorption as shown in Fig. 1. The peak at 780 K as shown in Fig. 2 (a) was related to the crystallization of

amorphous FeBSi, which released trapped He from the amorphous free volume [14]. In addition, the peaks at about 970 K and 1220 K were attributed to trapped He being released from interstitial-related and void-related defects in amorphous alloy and interstitial-type dislocation loops and voids in crystalline alloy, respectively. Similar to Fig. 1, desorption of mass 3 is also shown in Fig. 2. Desorption peak of mass 3 did not appear, although the background of it increased with increasing temperature.

Thermal desorption of masses 3 and 4 in amorphous alloy irradiated sequentially by 5 keV D₂ and He ions and 5 keV He and D₂ ions are shown in Fig. 3 (a) and (b), respectively. Thermal desorption spectrum of mass 4 was the same as He thermal desorption from amorphous irradiated by 5 keV He ions as shown in Fig. 2 (a) except the peak at temperature of 450 K. Compared with thermal desorption spectrum of mass 3, which is thought to come from HD, in samples irradiated by 5 keV D₂ and He and by only He as shown in Fig. 2 (a), the peak at temperature of 450 K came from release of D₂, since thermal desorption spectrum of mass 3 shows the peak at the same temperature although the peak was not remarkable. There is also an unclear peak of mass 4 and 3 in thermal desorption spectrum at temperature of 450 K in amorphous irradiated by 5 keV He and D₂ ions as shown in Fig. 3 (b). This peak is also thought to come from release of D₂. These results indicate that He irradiation induces sorption of D₂ in amorphous alloy. Defects can be produced in both irradiations with 5 keV He and D₂, which trap D atoms, and no D atoms trapped by interstitial or vacancy-related defects were released at temperature of 450 K as shown in Fig. 1. Thus, D₂ atoms came from the thermal desorption peak are not trapped by defects produced by He irradiation, they are bounded with He atoms. On the other hands, there is not peak of mass 3 at temperature higher than 900 K, therefore, the

peaks at high temperature are thought to come from release of He atoms. In other words, the effect of D₂ atoms on sorption of He in amorphous alloy is not predominant.

The desorption of masses 3 and 4 in crystalline alloy is the same as that in amorphous alloy as shown in Fig. 4 (a) and (b), where samples were irradiated sequentially by 5 keV D₂ and He ions and 5 keV He and D₂ ions, respectively. The peak at temperature of 400 K, which shifted to low temperature compared with that in amorphous alloy, is thought to come from D₂ release in both irradiations. The peaks at higher temperatures are thought to come from He release. These results also indicate that He irradiation influences D₂ sorption, however, D₂ irradiation does not affect He sorption in crystalline alloy.

H.T. Lee *et al.* reported that He retention and release were affected very little by the presence of D, but the presence of He enhanced D trapping in the near surface of W irradiated simultaneously by D and He [15]. They also indicated that D atoms were trapped possible at interstitial sites surrounding He-vacancy defects. Although the samples are different in our study, the results of the present study agree with those reported by H.T. Lee *et al.*. Geng *et al.* also supported that D atoms were trapped He-vacancy defects in W. They estimated the trapping energy to a substitutional He atom for the first H was as large as -0.96 eV [16].

4. Conclusion

Interaction of He and D in amorphous and crystalline FeBSi alloys was investigated by single irradiation with 5 keV He⁺ ions and 5 keV D₂⁺ ions, and double irradiations with 5 keV He⁺ + 5keV D₂⁺ ions and 5keV D₂⁺ + 5 keV He⁺ ions, respectively. Sorption of He atoms was more predominant than that of D atoms in both alloys under single irradiation

with 5 keV. Pre-irradiation with 5 keV D_2^+ ions did not influence the sorption of He atoms, on the other hand, pre-irradiation with 5 keV He^+ ions increased the sorption of D atoms.

References

- [1] P. Klaver, E. Haddeman and B. Thijssse, Nucl. Instrum. Methods B 153 (1999) 228.
- [2] W.D. Wilson and R.A. Johnson, Rare gases in metals, in interatomic Potentials and Simulation of Lattice Defects – Part 3, P.C. Gehlen, J.R. Beeler and R.I. Jaffee. eds., Plenum, New York, 1972, p. 375.
- [3] K. Ono, T. Kino, S. Furuno, K. Hojou, K. Izui, K. Mizuno and K. Ito, J. Nucl. Mater. 179-181 (1991) 978.
- [4] K. Niwase, T. Ezawa, T. Tanabe, M. Kiritani and F.E. Fujita, J. Nucl. Mater. 203 (1993) 56.
- [5] N. Yoshida, Radiation Effects & Defects in Solids, 148 (1999) 535.
- [6] Q. Xu, T. Yoshiie and K. Sato, J. Nucl. Mater. 386-388 (2009) 363.
- [7] H. Kawanishi, S. Ishino, ASTM-STP 1047 (1990) 179.
- [8] R.E. Gold, E.E. Bloom, F.W. Clinard, D.L. Smith, R.D. Stevenson, W.G. Wolfer, Nucl. Technol. Fusion 1 (1981) 169.
- [9] L.R. Greenwood, F.A. Garner, B.M. Oliver, J. Nucl. Mater. 212-215 (1994) 492.
- [10] F.A. Garner, M.L. Hamilton, L.R. Greenwood, J.F. Stubbins, B.M. Oliver, ASTM-STP 1175 (1992) 921.
- [11] T. Yamamoto, G.R. Odette, P. Miao, D.T. Hoelzer, J. Bentley, N. Hashimoto, H. Tanigawa, R.J. Kurtz, J. Nucl. Mater. 367-370 (2007) 399.
- [12] Z.X. Tian, W. Xiao, F.R. Wan and W.T. Geng, J. Nucl. Mater. 407 (2010) 200.
- [13] J.P. Biersack and L.G. Haggmark, Nucl. Instrum. Meth. 174 (1980) 257.
- [14] Q. Xu, X.Z. Cao, K. Sato, K. Mori and T. Yoshiie, Phil. Mag. Lett. 90 (2010) 131.
- [15] H.T. Lee, A.A. Haasz, J.W. Davis, R.G. Macaulay-Newcombe, D.G. Whyte and G.M. Wright, J. Nucl. Mater., 363-365 (2007) 898.

[16] B. Jiang, F.R. Wan and W.T. Geng, Phys. Rev. B 81 (2010) 134112.

Figure Captions

Fig. 1 D_2 thermal desorption in amorphous (a) and crystalline FeBSi (b) alloys after 5 keV D_2 irradiation to $1.0 \times 10^{20} D_2/m^2$.

Fig. 2 He thermal desorption in amorphous (a) and crystalline FeBSi (b) alloys after 5 keV He irradiation to $1.0 \times 10^{20} He/m^2$.

Fig. 3 Thermal desorption of masses 3 and 4 in amorphous FeBSi alloy sequentially irradiated by 5 keV D_2 and He ions (a) and 5 keV He and D_2 ions (b).

Fig. 4 Thermal desorption of masses 3 and 4 in crystalline FeBSi alloy sequentially irradiated by 5 keV D_2 and He ions (a) and 5 keV He and D_2 ions (b).

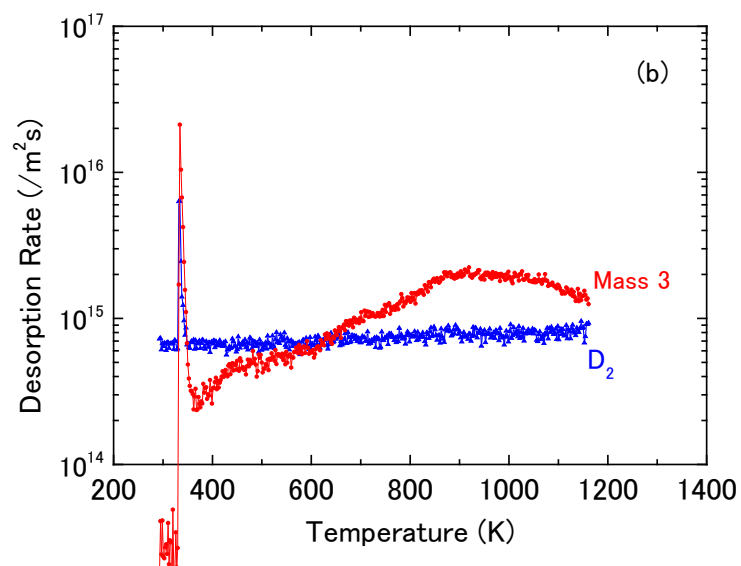
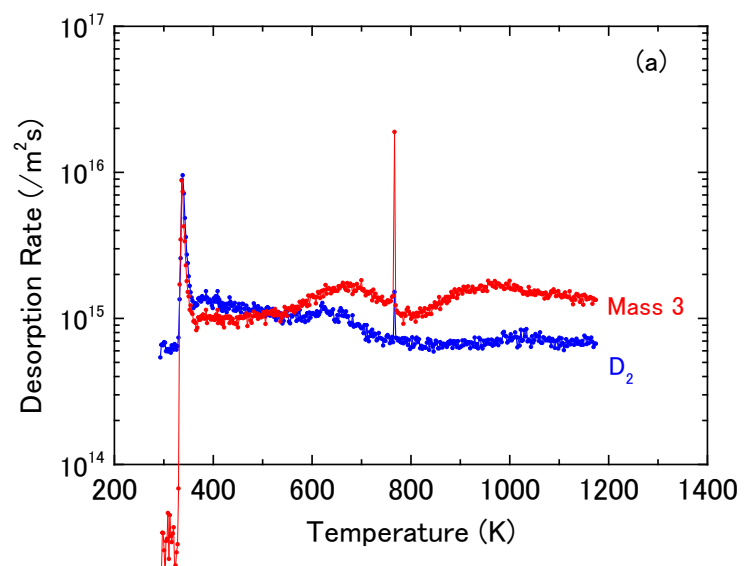


Fig. 1

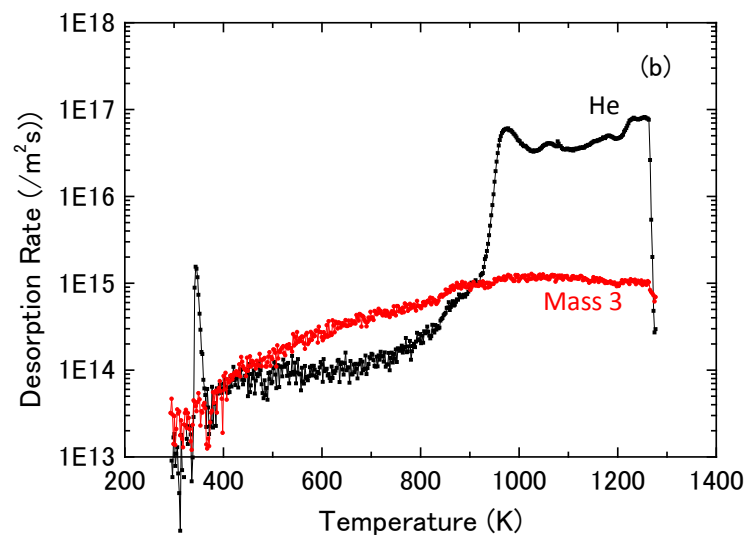
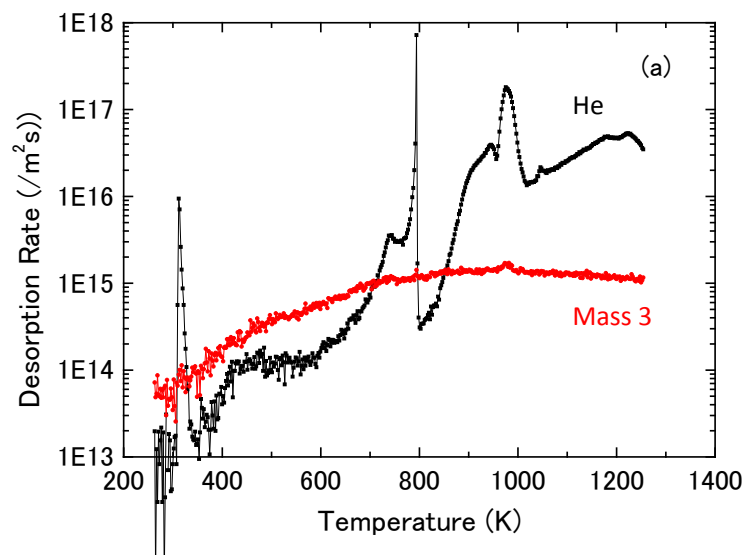


Fig. 2

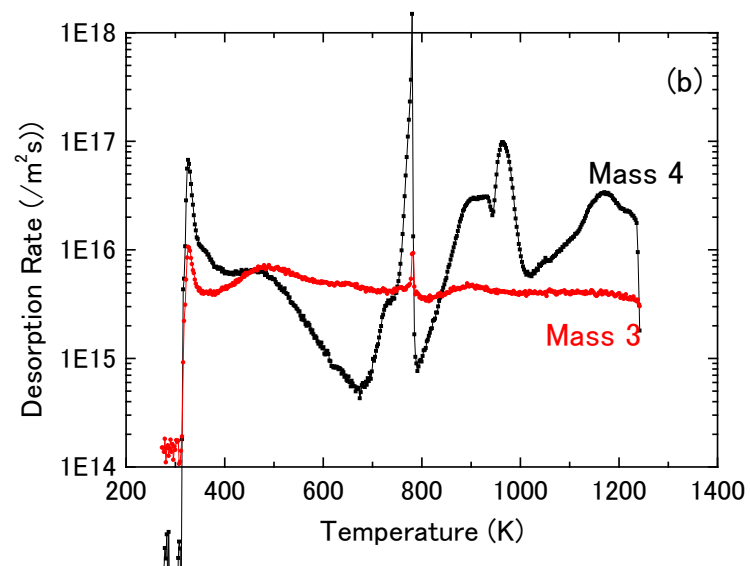
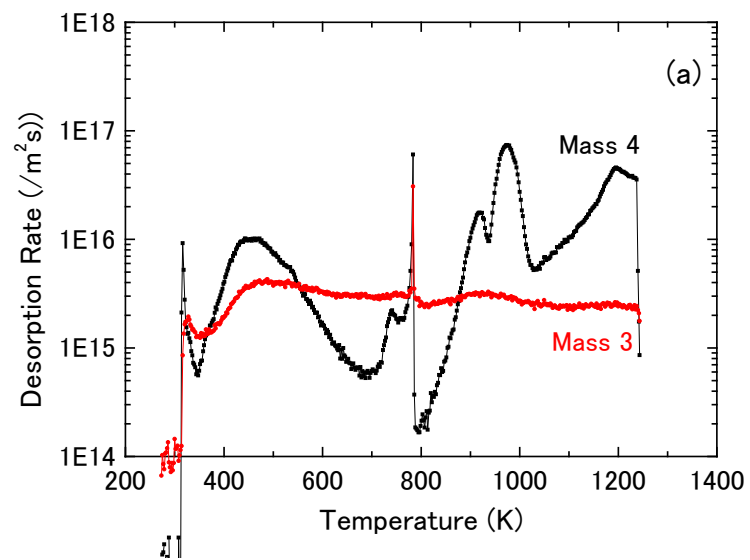


Fig. 3

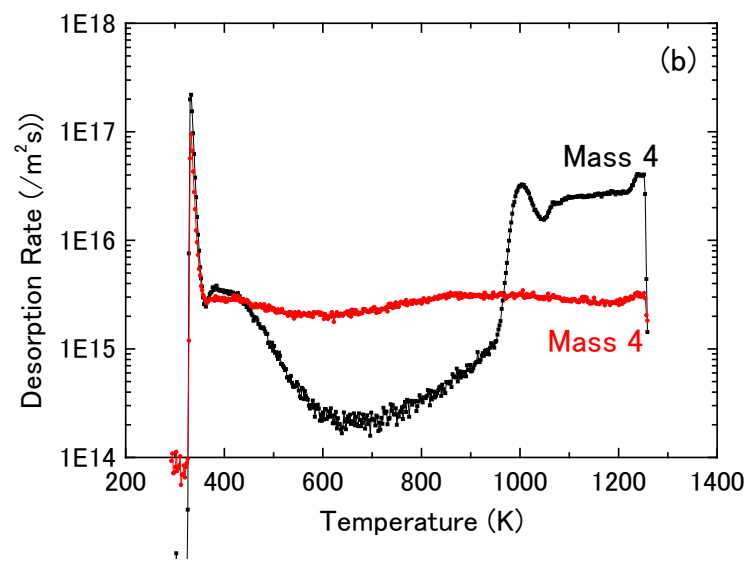
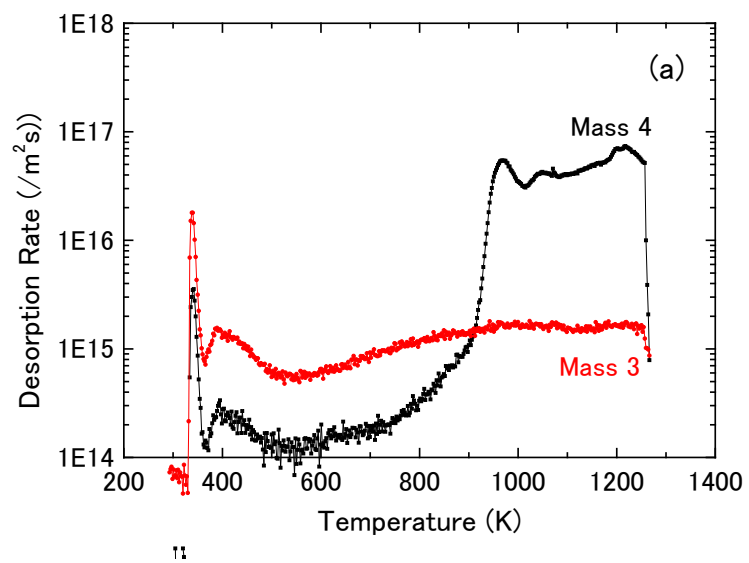


Fig. 4