A study of vacancy-type defects in amorphous and crystalline FeBSi alloys after He ion irradiation

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Abstract. In order investigate the structural dependence of defect formation during irradiation, amorphous Fe⁷⁹B¹⁶Si⁵ alloy and crystalline FeBSi alloy were irradiated by 300 keV helium ions at room temperature. Positron annihilation lifetimes observed for the unirradiated amorphous and the crystalline FeBSi alloys were nearly equal, i.e., 124.4 ± 0.3 ps and 124.6 ± 0.2 ps, respectively. The S parameters of the Doppler-broadening of annihilation radiation measured using a positron beam were also similar for the unirradiated amorphous and crystalline FeBSi alloys. It means that the positron annihilation at the free volume in amorphous Fe⁷⁹B¹⁶Si⁵ alloy is not prominent. The Doppler-broadening S parameter increased after the helium irradiation. This phenomenon was more pronounced in the amorphous FeBSi alloy. It suggests that the atoms are more easily displaced in amorphous alloy than in crystalline alloy during irradiation.

1. Introduction
With advances in nuclear power technology, in particular fusion reactor technology, interest in the behavior of He in solids has increased. In a fusion reactor, helium is introduced into materials at a high rate by direct implantation, but also indirectly, such as by the nuclear transmutation reaction of (n, α). Helium, which has a strong interaction with vacancies [1, 2], forms a high density of He bubbles. In a fusion reactor, helium and He bubbles lead to surface damage such as erosion, sputtering, and blistering of the plasma-facing materials (PFMs). The impurities induced by erosion of the PFMs are a key factor in the radiative power loss of the plasma. Therefore, it is important to find materials with low helium retention and/or better resistance to He bubble formation. The configuration of atoms is one factor influencing the retention of helium in solids, and amorphous metals have a very different atomic configuration from crystalline metals. Point defects and defect clusters are produced by irradiation with high energy particles in crystalline metals. Point defects and defect clusters, especially vacancies and voids, act as helium trapping sites. Although point defects and defect clusters do not exist in amorphous metals, helium atoms are also trapped during He irradiation. It would be interesting to clarify the helium trapping sites in amorphous metals.
The positron annihilation technique is a very powerful tool in the study of fundamental microstructural features, such as small vacancy-type defects, of localized sites in condensed matter [3], because the positron annihilation rate is proportional to the electron density around the annihilation site. Of course, energy and momentum are conserved in the positron annihilation process. In the dominant decay mode of a thermal positron and electron, two gamma rays are emitted. The energies of the two photons emitted by the annihilation of a positron and an electron are different. This difference in photon energy is proportional to the longitudinal component of the electron-positron momentum in the direction of gamma emission. Measurement of the photon energies reveals information regarding the momentum distribution of valence and core electrons. In the present study, defect formation and the interaction between defects and helium under He irradiation were investigated by positron annihilation analysis.

2. Experimental procedure

The amorphous alloy Fe$_{79}$B$_{16}$Si$_{5}$ (Metglas 2605S-3, The Nilaco Corporation (Japan)) was obtained in 25-µm-thick sheets. The crystallization temperature ($T_c$) was ~788 K. Crystalline FeBSi alloy specimens were prepared in a vacuum furnace by rapidly heating amorphous ribbons to 923 K and holding for 0.5 hours. Amorphous and crystalline samples were irradiated by 300 keV He$^+$ ions from a Van de Graaff accelerator at the University of Tokyo to $1\times10^{20}$ He/m$^2$ at room temperature. The damage induced by the ions in the matrix was not uniform, and the damage peak was about 800 nm from the irradiation surface, according to calculations using the TRIM code [4], as shown in Fig. 1. In order to investigate the irradiation depth dependence of microstructural evolution, the Doppler broadening of annihilation radiation measurements were performed using a mono-energetic positron beam apparatus combined with the Van de Graaff accelerator. Details of the apparatus used have been described previously [5]. The implantation profile of mono-energetic positrons into a material may be given by the following equation [6, 7]:

$$P(x, E) = -\frac{d}{dx} \exp(-x^m / x_0^m)$$

(1)
Here, $x_0=(\alpha/\rho)E^n$, $\rho$ is the material density in g/cm$^3$, $E$ is the incident positron energy in keV, and $x$ is the distance from the surface in cm. In the calculation of the positron implantation profile, we used the Makhovian parameters of $\alpha=4.0$ $\mu$g/cm$^2$/keV$^{-1.6}$, $m=2$, and $n=1.62$ determined by Vehanen et al [7]. Figure 2 shows implantation profiles of positrons with typical energies of 5, 10, 15, 20, 25, and 30 keV. The implantation profile of positrons is broadened gradually with increasing beam energy. At $E=20$ keV, most positrons are stopped within the damaged region formed by 300 keV He$^+$ ions.

![Figure 2](image)

Fig. 2 Depth profile of positron stopping probability for energies of 5, 10, 15, 20, 25 and 30 keV.

### 3. Results and discussion

The lifetime spectra were hardly decomposed into two components for the unirradiated amorphous or the crystalline FeBSi samples. Their mean lifetimes are 124.4 ± 0.3 and 124.6 ± 0.2 ps, respectively. Although free volume is introduced into amorphous alloy by rapid quench, the positron annihilation at the free volume is not prominent.

Figure 3 shows the dependence of the $S$ parameter for the amorphous and the crystalline FeBSi samples before and after the He irradiation as a incident positron beam energy. In both the unirradiated amorphous and the crystalline FeBSi samples, the $S$ parameter decreased with increasing positron energy up to 5 keV, and then became constant. The high $S$ parameter at low incident positron energies comes from the positron diffusion to the surface and consequent production of ortho-positronium [8, 9]. Huomo et al. indicated that positrons with energy lower than 4 keV diffuse back to the surface in Mo [10]. The fraction of positrons diffusing back to the surface decreases at high incident positron energies. Before the He irradiation, the $S$ parameters for the amorphous and the crystalline FeBSi samples are nearly the same when the positron energy is higher than 8 keV. This is consistent with the above-mentioned positron lifetime measurements. Thus, there are no important differences in the positron annihilation mechanisms in the amorphous and the crystalline FeBSi samples. After the He irradiation, on the other hand, the $S$ parameters of both the amorphous and the crystalline FeBSi samples increase as the incident positron energy increases from 0 to 2 keV, and then decrease to constants with increasing the incident positron energy. The high $S$ parameters at around $E=2$ keV are probably due to defects produced near the surface, which trap positrons to suppress the fraction of positrons diffusing back to the surface. The diffusion of positrons back to the surface is negligible.
above $E = 5$ keV. Thus, the change of $S$ parameter above $E = 5$ keV reflects some structural change in the bulk. After the He irradiation, the $S$ parameters of the crystalline FeBSi sample increases. This indicates the introduction of vacancy-type defects due to atomic displacement in the FeBSi matrix. The $S$ parameter of the amorphous FeBSi sample further increases. Thus, vacancy-type defects that can trap positrons are also produced in the amorphous FeBSi structure [11]. Moreover, vacancy-type defects are more easily produced in amorphous FeBSi than in crystalline FeBSi by He irradiation. This may indicate that comparing the crystal phase in the amorphous phase the displacement energy is lower possibly due to the weaker binding energy between atoms.

![Fig. 3 Dependence of the S parameter on incident positron energy for the amorphous and crystalline FeBSi samples before and after the He irradiation.](image)

4. Conclusion

Amorphous and crystalline FeBSi alloys irradiated with 300 keV He ion were studied by positron annihilation spectroscopy. Vacancy-type defects acting as positron trapping centers are formed in both amorphous and crystalline FeBSi alloys by He irradiation, while the production of vacancy-type defects is enhanced in the amorphous alloy.

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