Lattice Structure Transformation of NiTi Intermetallic Compound Induced by Energetic Ion Bombardment

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1 Introduction

NiTi shape memory alloys exhibit various lattice structure transformations under some extreme conditions. For example, an amorphous NiTi alloy was obtained by the high-pressure torsion [1] and by the mechanical alloying[2]. In addition, a lot of studies on the effects of energetic particle (electron or ion) irradiation on the lattice structures of NiTi alloy have been reported[3-9]. Most of the previous studies have, however, been performed by using only one particle species in narrow ion energy ranges. To clarify the effect of energetic particle irradiation on the lattice structure of NiTi samples, it is necessary to perform more systematic irradiation experiments by using a wide range of irradiation parameters on the same kind of target. Moreover, most of the previous experiments have been performed by using thin films for the TEM observations. Effects of charged particle irradiation in thin films are possibly influenced by the sample surfaces, which act as strong sinks against irradiation-produced lattice defects.

In the present study, Ni-50.8%Ti intermetallic compound was used as a target material. The NiTi bulk samples were irradiated with 16MeV Au ions, or 200MeV Xe ions at room temperature. From the change in the grazing angle x-ray diffraction (GIXD) spectrum and the extended x-ray absorption fine structure (EXAFS) spectrum for each ion species and ion fluence, we have discussed the contribution of elastic collisions (or the displacements per atoms (dpa)), and the electronic excitation to the irradiation-induced lattice structure transformation.

2 Experiment

A Ni-50.8% Ti intermetallic compound was prepared from starting raw materials of 99.9 wt.% Ni, and 99.9 wt.% Ti. After the homogenization treatment, the ingot button was cut into several sheets with a dimension of 10 \times 10 \times 1 mm³. The sheets were irradiated at room temperature with 16 MeV ¹⁹⁷Au⁵⁺ ions or 200MeV ¹³⁶Xe¹⁴⁺ ions. As the projected ranges of these ions are 2-10 µm, the energy depositions by the both ion irradiation are restricted only near the surface region. Therefore, we have used the grazing incidence CuK x-ray diffraction (GIXD) with the incident angle of 0.5 degree to estimate the change in surface lattice structures accurately. For such a diffraction condition, the attenuation length of the CuKa x-ray is about 100 nm[10], and therefore, the GIXD spectra show the lattice structure from the surface to the depth of about 100 nm. To estimate the ion irradiation effects on the local atomic arrangements around Ti atoms, the EXAFS measurement was performed at the 27B beam line of the Photon Factory. The EXAFS spectra were obtained near the Ti K-edge (X-ray energy of 4965 eV) at room temperature. We performed the EXAFS measurement for the unirradiated sample, the Xe ion irradiated sample (fluence; $5x10^{13}$ /cm²) and the Au ion irradiated sample (fluence; $5x10^{14}$ /cm²).

3 <u>Results and Discussion</u>

In Fig.1, the GIXD spectrum for the unirradated NiTi sample is shown. Most of the diffraction peaks for the unirradiated sample can be identified as those of the B19³ lattice structure, and other peaks are identified as those of the B2 structures. The transition temperature of NiTi alloy between the high temperature ordered structure (B2) and the low temperature (B19') structure is close to the room temperature, and it strongly depends on the thermal treatment of the samples. The spectrum for the unirradiated sample implies that the mixture of the B19' and B2 structures is obtained by the thermal treatment in the present experiment. In Fig.2, the GIXD spectra for the samples irradiated with 200MeV Xe ions are shown. By the Xe irradiation above the fluence of 1×10^{13} /cm², narrow peaks corresponding to the A2 structure, in which Ni atoms and Ti atoms are randomly distributed at the BCC lattice sites, appear, but any peaks for the B2 structure or the B19' structure can scarcely be found. The result indicates that the lattice structure is completely transformed to the A2 structure by the 200MeV Xe ion irradiation. Fig. 3 shows the GIXD spectra for the NiTi samples irradiated with 16MeV Au ions. After the Au ion irradiation with the fluence up to 2.5×10^{12} /cm², the spectra are about the same as that for the unirradiated sample, i.e the peaks corresponding to B19' and B2 structures are still observed. For the Au fluence of 5x10¹³/cm², a largely broadened peak around 42 degree dominates the spectrum. The present result implies that the lattice structure tends to be amorphized by the16MeV Au ion irradiation with higher ion fluences. Fig. 4 shows

the EXAFS-FT spectrum near the Ti K-edge for 200MeV Xe ion irradiation with the fluence of $5x10^{13}$ /cm² and that for 16MeV Au ion irradiation with the fluence of $5x10^{14}$ /cm². The spectrum for the unirradiated sample is also shown. As compared with the spectrum for the unirradiated sample, in the EXAFS spectrum for the Au irradiation, only a peak around 2.4 A, which corresponds to the nearest neighbor atoms of Ti atom is clearly observed, and other peaks are quite small or can hardly be observed. This EXAFS result confirms that the sample was mostly amorphized by the Au ion irradiation. On the other hand, in the EXAFS-FT spectrum for the 200MeV Xe ion irradiation, some peaks can also be observed as well as a large peak around 2.4A, suggesting that the sample irradiated with the Xe ions is not amorphized but has some lattice structure. This result is consistent with the result of the GIXD measurement. To compare the irradiation effects on materials, the value of dpa (displacements per atom) has often been used. The value of dpa means the number of atomic displacements by the elastic interaction between irradiating particles and target atoms. Here, we compare the GIXD result for 200MeV Xe ion irradiation (ion fluence, $1x10^{13}/cm^2$) with that for 16MeV Au ion irradiation (ion fluence, $1x10^{12}/cm^2$). Although the value of dpa for the Xe ion irradiation $(1.4x10^{-3})$ is smaller than that for the Au ion irradiation (2.3×10^{-3}) , the GIXD spectrum strongly changes by the Xe ion irradiation, and the A2 structure is induced by the Xe irradiation. On the other hand, for the Au ion irradiation, the change in GIXD spectrum can scarcely be observed. The present result shows that the lattice transformation from the B19' structure to the A2 structure by the Xe irradiation can be attributed the high density electronic excitation by the 200MeV Xe ions.



Fig. 1: GIXD spectrum for unirradiated NiTi sample.

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Fig.2 GIXD spectra for NiTi samples irradiated with 200MeV Xe ions. (blue) unirradiated, (red) $1x10^{13}$ /cm², (green) $2x10^{13}$ /cm², (black) $5x10^{13}$ /cm², and (brown) $1x10^{14}$ /cm².



Fig.3 GIXD spectra for NiTi samples irradiated with 16MeV Au ions. (blue) unirradiated, (red) 1×10^{11} /cm², (green) 5×10^{11} /cm², (brown) 1×10^{12} /cm², (pink) 2.5×10^{12} /cm² and (sky blue) 5×10^{13} /cm².



Fig. 4 EXAFS –FT spectra for unirradiated NiTi, Xe ion irradiated NiTi and Au ion irradiated NiTi. Ion fluence is $5x10^{13}$ /cm² for Xe ion irradiation and $5x10^{14}$ /cm² for Au ion irradiation..

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