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Effect of elastic collisions and electronic excitation on lattice structure of NiTi bulk intermetallic compound irradiated with energetic ions

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ABSTRACT

NiTi bulk intermetallic compound with the B19′ structure was irradiated with 1 MeV He, 5 MeV Al, 16 MeV Au and 200 MeV Xe ions, and the change in lattice structure near the surface by the ion bombardment was investigated by using the grazing incidence X-ray diffraction (GIXD) and the extended X-ray absorption fine structure (EXAFS). The lattice structure transformation by the irradiation strongly depends on ion species and/or energies. For the 1 MeV He irradiation, the lattice structure changed from B19′ to the A2 structure, but did not show an amorphization even after the high fluence irradiation. For the 5 MeV Al irradiation, the samples are partially amorphized. For the 16 MeV Au irradiation, the lattice structure of the NiTi samples changed nearly completely from the B19′ structure to the amorphous state via the A2 structure. The value of dpa (displacement per atom) which is needed for the amorphization is, however, much smaller than the case of the Al ion irradiation. For the 200 MeV Xe ion irradiation, the lattice structure completely changed to the A2 structure even by a small ion fluence. The dependence of the lattice structure transformation on elastic collisions (dpa), the spectrum of the primary knock-on (PKA) atoms and the density of energy deposited through electronic excitation was discussed.

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 during the synthesis of NiTi alloy from Ni and Ti pure metals by using the mechanical alloying, lattice structures of B19′, B2 and amorphous phases appear, depending on the milling time [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. The observation by the transmission electron microscope (TEM) have shown the electron beam induced amorphization in NiTi thin films [3,4]. Watanabe et al. have reported that for the irradiation dose less than 0.16 dpa, the electron irradiation induces the chemical disordering and the lattice structure changes from the B2 (ordered) structure to the A2 (disordered BCC) structure and that for the irradiation dose above 0.25 dpa, the NiTi samples are completely amorphized. The amorphization and other lattice structure transformations have also been observed in energetic ion irradiated NiTi samples [5–9]. The direct transition from the B19′ phase to the amorphous phase has been observed without going through the ordered (B2) phase in NiTi samples irradiated with 2 MeV H ions at low temperatures (120 K and 230 K) [5] and those irradiated with 380 keV Ni ions [6]. Some papers show that the electronic excitation plays an important role in the lattice phase transition of NiTi during high energy heavy ion irradiation [7–9]. For the irradiation with the electronic stopping power, $S_e > 46$ keV/nm, the amorphous tracks are observed in B19′ NiTi samples, but for the irradiation with the S_e value below 17 keV/nm, no S_e effects are observed [8]. While on the other hand, the S_e effect is observed in NiTi sample irradiated with 5 MeV Ni ions, the S_e value of which is less than 17 keV/nm [9]. Such previous studies have, however, been performed by using a few kinds of ion 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 studies, have reported experimental

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results 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. Recently, by using various ion species and energies, we have performed ion irradiation experiments for some bulk intermetallic compounds, and have discussed the irradiation effects not only on lattice structures but also on macroscopic properties such as magnetic and mechanical properties [10–19], which can hardly be studied for thin film samples.

In the present study, Ni-50.8%Ti intermetallic compound was used as a target material. The NiTi samples were irradiated with 1 MeV He ions, 5 MeV Al ions, 16 MeV Au ions, or 200 MeV Xe ions at room temperature. From the change in the grazing angle X-ray diffraction (GIXD) spectra 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. To confirm the lattice structure transformation by Xe and Au ion irradiations, the extended X-ray absorption fine structure (EXAFS) spectra were measured by using a synchrotron radiation facility. The dependence of the lattice transformation on the PKA energy spectrum was discussed in this report.

2. Experimental procedure

A Ni-50.8%Ti intermetallic compound was prepared from starting raw materials of 99.9 wt%Ni, and 99.9 wt%Ti. A button ingot was made by arc melting in an argon gas atmosphere. The ingot button was annealed at 973 K for 30 min and cooled to room temperature. After homogenization, the ingot button was cut into several sheets with a dimension of $10 \times 10 \times 1\ mm^3$. The sheets were irradiated at room temperature with 5 MeV $^{27}Al^{3+}$ ions or 16 MeV $^{197}Au^{5+}$ ions by using a tandem accelerator at Takasaki Advanced Radiation Research Institute, Institutes for Quantum and Radiological Science and Technology (QST-Takasaki). Other samples were also irradiated at room temperature with 1 MeV $^{4}He^{+}$ ions by using a single-ended accelerator at QST-Takasaki. We irradiated some samples with 200 MeV $^{136}Xe^{14+}$ ions by using a tandem accelerator at Nuclear Science Research Institute, Japan Atomic Energy Agency.

Fig. 1 shows the depth profiles of the energy deposited through the elastic collisions and through the electronic excitation by one ion per unit path length (i.e., the nuclear stopping power, S_n, and the electronic stopping power, S_e, respectively) for 1 MeV ^{4}He, 5 MeV ^{27}Al, 16 MeV ^{197}Au, and 200 MeV ^{136}Xe ion in the Ni-50.8%Ti target. The profiles were calculated by using the SRIM code (full cascade mode) [20]. For the calculation of the depth profiles, we used the value of 6.46 g/cm^3 as the density of the NiTi target. The figure shows that the both energy depositions by the ion irradiation are restricted only near the surface region except for the Xe ion irradiation. Therefore, we have used the grazing incidence CuKα 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 penetration depth of the CuKα X-ray is about 100 nm [21], and therefore, the GIXD spectra show the lattice structure from the surface to the depth of about 100 nm. The irradiation parameters (ion species, ion energies, ion ranges, electronic and nuclear stopping powers) for the present experiment are summarized in Table 1. The values of $\langle S_e \rangle$ and $\langle S_n \rangle$ in Table 1 mean the averaged values from the surface to the depth of 100 nm.

In the table, we also show the cross section of the defect production by the elastic collisions, σ_d, near the sample surface, which were calculated by using the SRIM code with 40 eV and 30 eV as the displacement threshold energy for Ni and Ti, respectively [22]. The value of displacements per atom (dpa) can be calculated by the following equation,

$$dpa = \sigma_d \Phi, \quad (1)$$

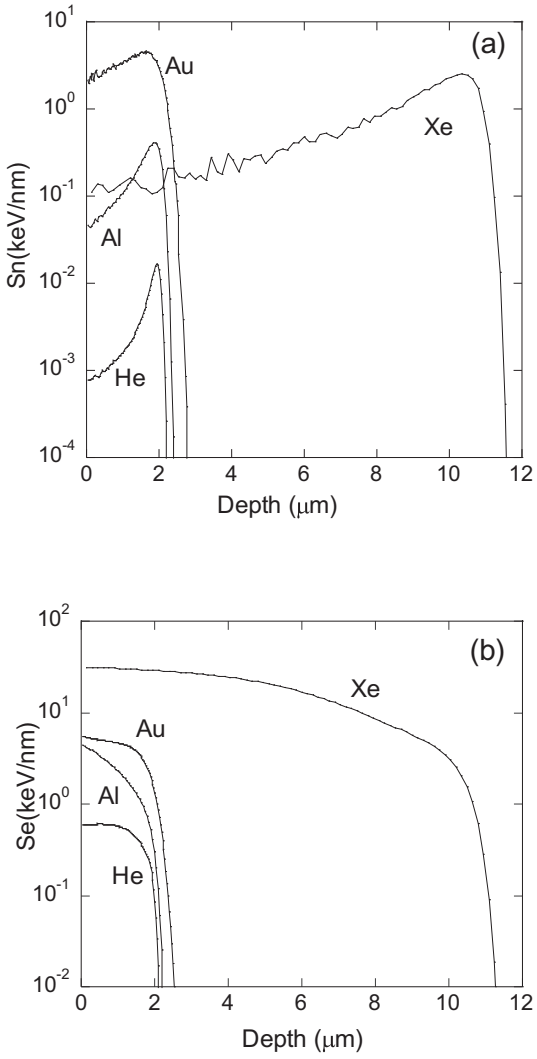

Fig. 1. Depth profile of (a) the nuclear stopping power, S_n, and the electronic stopping power, S_e for 1 MeV He ion, 5 MeV Al ion, 16 MeV Au ion and 200 MeV Xe ion.

Table 1
Irradiation parameters.

Ion species	Energy (MeV)	Projected range (μm)	$\langle S_e \rangle$ (keV/nm)	$\langle S_n \rangle$ (keV/nm)	σ_d (cm^2)
^{4}He	1.0	1.95	0.589	7.56×10^{-4}	1.92×10^{-18}
^{27}Al	5.0	1.93	4.14	4.42×10^{-2}	7.52×10^{-17}
^{197}Au	16.0	1.92	5.44	2.35	2.46×10^{-15}
^{136}Xe	200	10.44	31.5	0.119	1.57×10^{-16}

where, Φ is the ion fluence.

To estimate the ion irradiation effects on the local atomic arrangements around Ni atoms, the EXAFS measurement was performed at the 27B beam line of the Photon Factory of High Energy Accelerator Research Organization (KEK-PF). The EXAFS spectra were obtained near the Ni K-edge (X-ray energy of 8332 eV) at room temperature. As the beam-time for the EXAFS measurement was strongly limited, we performed the measurements only for unirradiated sample, the sample irradiated with 200 MeV Xe and that irradiated with 16 MeV Au ions.