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Structural analysis of $Ti_{50}Ni_{44}Fe_6$ single crystal by X-ray fluorescence holography

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Introduction

Ti-Ni alloy with 6 at. % iron shows second-order-like parent-incommensurate-commensurate transitions [1,2], and anomalies in some physical properties at low temperatures. X-ray fluorescence holography (XFH) is a novel technique to experimentally visualize three dimensional (3D) atomic arrangements [3] around fluorescing atoms in single crystals. To clarify the changes of atomic position by the phase transition, we applied the XFH technique to the $Ti_{50}Ni_{44}Fe_6$ single crystal. Holograms were recorded at 225 K and 100 K, where the parent and commensurate phases appear, respectively and the 3D atomic images around the Fe atoms were successfully reconstructed. In present study, structural change due to phase transition and the difference of atomic images in two phases are discussed.

Experimental

Single-crystalline rods of the $Ti_{50}Ni_{44}Fe_6$ alloys were grown by a floating zone method with a growth rate of 10 mm/h. The XFH experiment was carried out at beamline BL6C of Photon Factory in KEK. The incident X-ray energies were 8.0-12.0 keV in steps of 0.5 keV. Using the toroidally bent graphite crystal, Fe K_α fluorescent X-rays from the sample were energy-analyzed and focused on avalanche photodiode detector (APD). Variations of the fluorescence intensities were recorded by scanning an azimuthal angle of the sample ϕ and the incident angle θ with the ranges of $0^\circ \le \phi \le 360^\circ$ and $0^\circ \le \theta \le 70^\circ$. X-ray exit angle was fixed at 60°. The dwelling time for each measurement was 1 sec in 1° step for both of ϕ and θ. The measurement time for one energy hologram was about seven hours.

Results and Discussion

Figures 1(a) and (b) show real space images of the (001) lattice plane at z = 0 Å of parent and commensurate phases, respectively. From the crystallographic knowledge of $Ti_{50}Ni_{44}Fe_6$ single crystal, it is found that images of neighboring Ni/Fe atoms were successfully visualized. Crosses of dotted lines indicate ideal atomic positions of Ni or Fe. Since the Fe atoms substitute for the Ni atoms, the Ni and Fe atoms exist in the same lattice plane. Comparison of atomic images between 100 K and 225 K suggests a short range structure of bcc and an additional fcc structure, the latter of which exists only in the commensurate phase. Further improvement of the XFH analysis will be carried out.

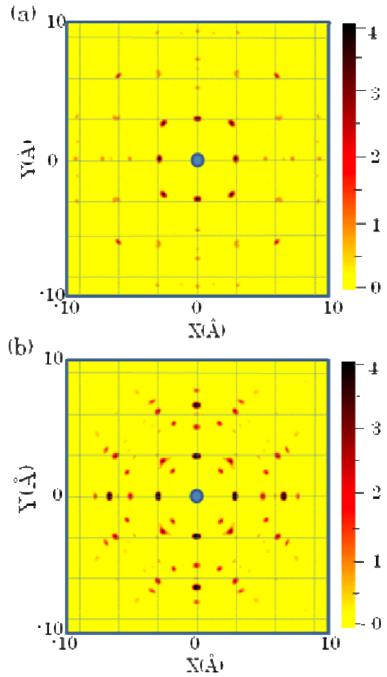

Fig. 1. Reconstructed real space images of the Ni or Fe atoms around Fe emitters (a) at 225K and (b) 100K. Reconstructed images parallel to the (001) lattice plane at z = 0 Å of parent and commensurate phases, respectively. Central spot correspond to the Fe emitter.

References

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