

Precursor Phenomena on the First-Order Phase Transition in Ferroelastic Compounds II

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Introduction

The ferroelastic compounds NdNbO_4 and LaNbO_4 transform from a high-temperature tetragonal phase ($I4_1/a$) into a low-temperature monoclinic phase ($I2/a$). Associated with these first-order phase transitions, precursor phenomena such as anomalous intensity-decreasing and profile-broadening on the X-ray Bragg reflections are found over a wide temperature range.^{1,2)} Anisotropic diffuse scattering around the Bragg reflections is also observed above the phase transition temperature T_c .

In the first experiment at SPring-8 in 1997, we confirmed the previous results of the precursor phenomena of LaNbO_4 by means of high-energy X-ray diffraction. In this study, we investigated the origin of the anisotropic diffuse scattering.

Experimental

X-ray diffraction studies were performed on the seven-axis diffractometer installed at the Crystal Structure Analysis beam-line (BL02B1) in SPring-8. A single crystal of NdNbO_4 was used to measure the diffuse scattering. A vacuum-furnace with a hemisphere-type Be-window was used to heat the sample up to 1100K on the diffractometer. The energy of X-ray used was 30keV monochromated by Si111 double crystals.

Results and Discussion

Intensity distribution of the diffuse scattering was measured around several Bragg reflections at 980K (cf. $T_c=930\text{K}$). Figure 1 shows the intensity map around $(0, 4, 0)$ reciprocal lattice point. As shown in the figure, the diffuse scattering extended to the

directions deviated from the crystal axes by 20° in the $(h k 0)$ tetragonal plane. The origin of the diffuse scattering is considered the phonon softening of the transverse acoustic mode at the Brillouin zone center. The deviation is caused by the low symmetry of the tetragonal phase with $4/m$ point group, i.e. without m_x and m_y symmetries. The propagating direction of the soft phonon coincides with the orientation of the domain boundary in the monoclinic phase.

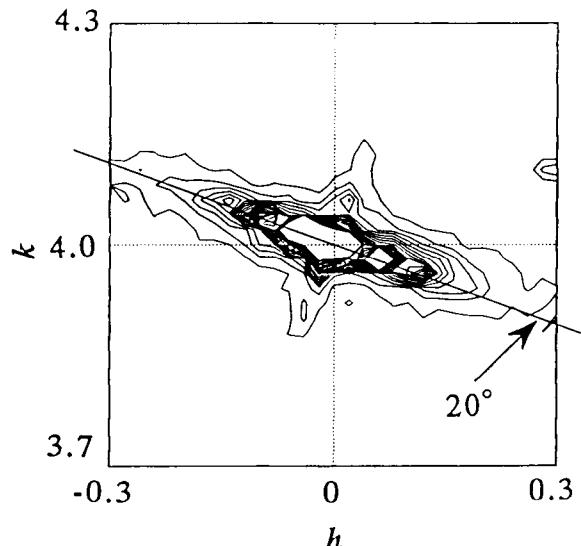


Fig.1 Anisotropic diffuse scattering around 040 Bragg reflection.

References

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