Investigation of the local crystal distortion in the relaxor ferroelectric (1-x)Pb($Mg_{1/3}Nb_{2/3}$)O_3-$x$$PbTiO_3$ ($0.0 \leq x \leq 0.40$) using extinction effect

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Relaxor ferroelectrics of the form $PbBB'O_3$ are receiving a great deal of scientific attention as a result of the extremely high piezoelectric response over a wide temperature range. The key concept to understand the relaxor behavior is believed to be the so-called polar nanoregions (PNR) at temperatures much above T_c. However, these clusters cannot be detected from the profiles of the X-ray and neutron diffraction Bragg peaks due to their extremely small size. In a nearly perfect crystal, the scattering intensity of a strong Bragg peak becomes smaller than the calculated value due to scattering by various crystallites, which is called secondary extinction. To elucidate the evolution of the PNR in the relaxor system, we investigated the thermal variations of Bragg peaks in the relaxor ferroelectric (1-x)Pb($Mg_{1/3}Nb_{2/3}$)O_3-$x$$PbTiO_3$ (PMN-xPT; $x = 0.0, 0.10, 0.20$, and 0.40) which could be associated with the thermal variation of the local crystal distortion by the secondary extinction effect. Neutron scattering experiments were performed on the triple-axis spectrometers PONTA installed at the JRR-3 Reactor of the JAEA.

Figure 1 (a) shows the temperature dependence of the integrated intensity at the (200) Bragg peak for PMN-10%PT. The peak intensity increases sharply at $T = 615$ and 280 K, which could be explained by a release of the secondary extinction effect due to the tilt of the crystal mosaics. Figure 1 (b) shows zero field phase diagram of PMN-xPT. Open circles denote the value of the *local* T_C at which a structural phase transition was observed by x-ray diffraction, but not by neutron diffraction. A bulk structural phase transition, however, was observed for $x \geq 0.27$, shown by closed circles. The higher temperature of the rapid increase in the (200) Bragg (T_d extinction: open rectangles) corresponds to the onset of the diffuse scattering, which can be associated with an appearance of PNR. The lower one (T_c extinction: open triangles) matches the structural phase transition temperature, which could be associated with an ordering of PNR. Both temperatures increases with PT substitution. In addition, the difference between these temperatures becomes small with x, which is expected to be zero at $PbTiO_3$.

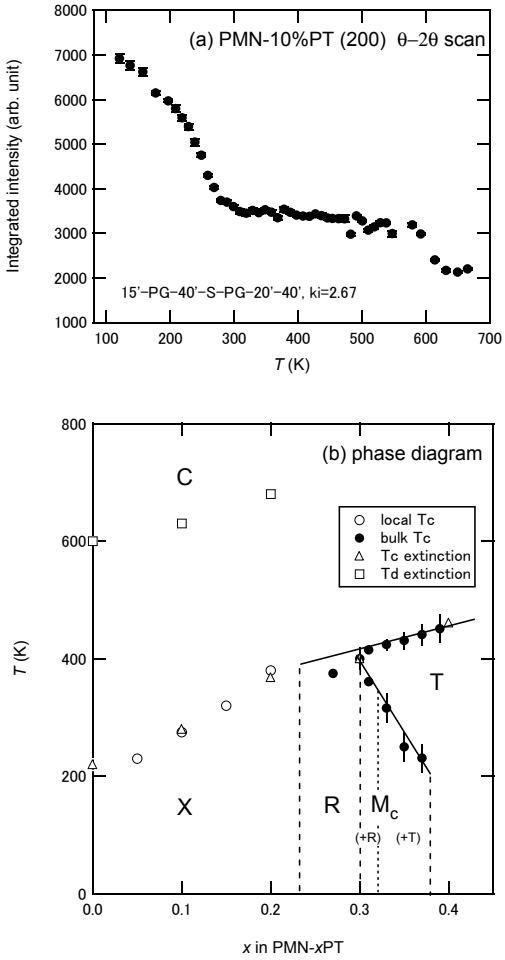

Fig. 1. (a) The temperature dependence of the (200) Bragg peak. (b) Zero field phase diagram of PMN-xPT.