Nature of Atomic Disordering in Relaxor Ferroelectrics of PMN and PSN

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A relaxor is a type of ferroelectrics whose crystal structure is given by a simple cubic perovskite often represented by ABO_3, where A is Pb^{2+}, and B consists of two different ionic species with their concentrations giving an averaged valence of 4+. The two systems which we have investigated, $Pb(Mg_{1/3}Nb_{2/3})O_3$ and $Pb(Sc_{1/2}Nb_{1/2})O_3$ (called PMN and PSN, respectively), have the ratios of 1:2 and 1:1, and the B-site ionic arrangements in the two systems are disordered. Because of this atomic nature, relaxors reveal a diffuse phase transition and dielectric dispersion. Therefore, for thorough understanding the mechanism it is very important to know basic features of the atomic disorder.

The powder patterns were taken at 700 K down to 200 K on PMN, and at 298 and 470 K on PSN (The transition temperatures for the two systems are around 273K and 353K, respectively.). An x-ray energy used is 30 keV. At this high energy, the x-ray does not suffer much absorption. FIG. 1 shows the typical pattern of PMN at 700K. Intensities of the peaks are found to follow a **Q** dependence of the static crystal structure factor for this system, i.e., a Bragg reflection exhibits the relatively high intensity if a sum of the three index digits, h+k+l, is an even integer, but not otherwise. Intensities of these peaks are reduced as temperature is lowered. The reduction is most likely to be caused by phonon softening toward the transition, and gives increase of background intensities as shown in FIG. 2. However, the two different temperature dependences of the peaks appear on cooling; one is significant, and the other not. The former case is seen for the odd-integer reflections, and the latter case for those with even integers. FIG. 3 displays the two representative plots for the (100) and (110) reflections. The difference in the trends results from development of the optic-mode distortions (which have already known to be of the transverse mode), since the atomic shifts which show their antiparallel orderes are more effective to the reduction for the odd-integer reflections.

Below room temperature, the intensities are still lowered, but the decrease is rather saturated. The other system, PSN, exhibits results which are quite similar to those for PMN. A further study on this topic is ongoing.

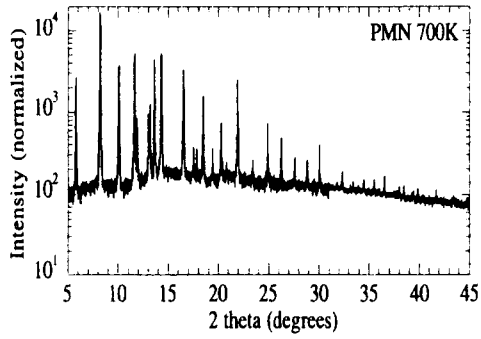

FIG. 1 Powder pattern of PMN at 700K.

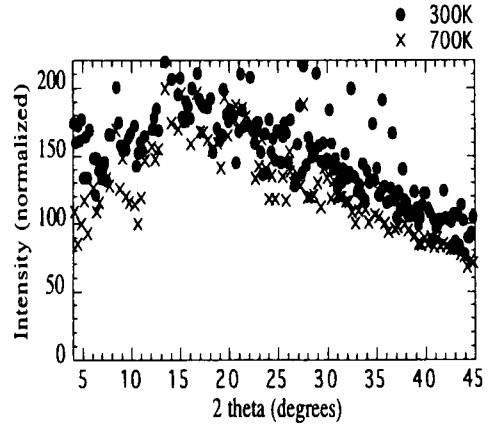

FIG. 2 Background intensities.

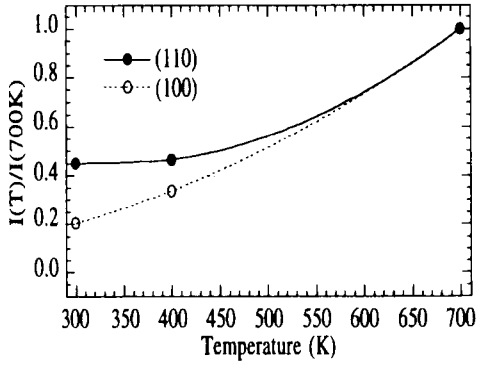

FIG. 3 (100) and (110) peak intensities.