Long- and short-ranged structure of multiferroic $Pb(Fe_{0.5}Nb_{0.5})O_3$

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Lead iron niobate $Pb(Fe_{0.5}Nb_{0.5})O_3$ (PFN) is a multiferroic disordered system. It has a G-type antiferromagnetic transition at T_N = 143 K and a ferroelectric transition at T_C = 385 K. Its reported high dielectric constant makes it a suitable candidate material for multilayer ceramic capacitors as well as other electronic devices. Despite the interesting properties, however there is still controversy over the room temperature structure: for example, two competing space groups of R3m and Cm structure have been so far proposed. More importantly, it is not clear whether this material has Pb-disorder. More recently, it was reported to have interesting negative thermal expansion behavior below the antiferromagnetic transition.

In order to understand the properties better and resolve some of the controversies, we carried out both high resolution neutron powder diffraction and total scattering experiments using S-HRPD and NOVA beamlines of J-PARC, respectively. By taking advantage of the data, we could analyze both long-ranged and short-ranged structures systematically.

For example, we found that there is no negative thermal expansion behavior below the antiferromagnetic transition by carefully examining the S-HRPD data. Our high resolution S-HRPD data also showed that the thermal parameter of Pb ion is unusually large, indicative of the existence of static disorder at the Pb site. This observation is corroborated by our total scattering analysis using the NOVA data.