Atomic pair-distribution function analysis on ferroelectric materials using synchrotron X-ray

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Since the domain structure exists in a ferroelectric material, there is a difference in average structure and local structure inside a domain. In a solid solution system from which average structure tends to be cubic structure, in order to understand a ferroelectric mechanism, a local structure analysis is required. We performed atomic pair-distribution function (PDF) [1] to resolve atomic bond distribution in nano scale order.

PDF analysis and X-ray absorption fine structure (XAFS) have been performed on samples in the mixture of $(BaTiO_3)_{0.5} - (KNbO_3)_{0.5}$. $BaTiO_3$ and $KNbO_3$ have the same phase transition sequence and almost same lattice parameters. Figure 1 shows the obtained PDFs of pure $BaTiO_3$ and $KNbO_3$. These local structures of $BaTiO_3$ and $KNbO_3$ are similar very well. The local structure is reflecting not only a ferroelectric interaction but also an elastic correlation and an excluded volume effect. These interactions can be extracted by combining and collaborating with the PDF analysis, traditional crystal structure analysis, and XAFS measurements.

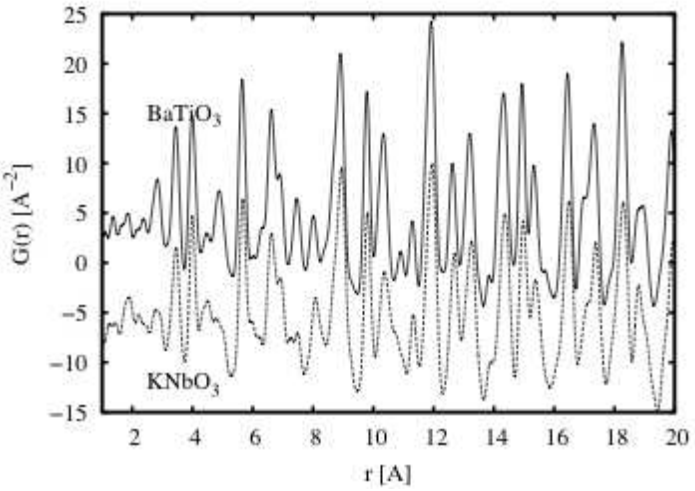

Fig. 1 Observed PDFs for pure $BaTiO_3$ and $KNbO_3$.

References

1. T. Egami and S. J. L. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials: Pergamon Press (2003)