10B, 14A/2001G080

Local structures of ordered and disordered $Pb(In_{1/2}Nb_{1/2})O_3$ studied by EXAFS

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Introduction

Extremely large dielectricity and piezoelectricity of "relaxor" ferroelectrics has been under discussion for almost half a century since the Smolenskii's discovery[1]. Typical relaxors are separated into two kinds of complex perovskites, $Pb(B'^{+2}_{1/3}B''^{+5}_{2/3})O_3$ and $Pb(B'^{+3}_{1/2}B''^{+5}_{1/2})O_3$. They exhibit distinct features of the chemical order for B-site cations, but in common form a heterogeneous structure including the nano-scale ordered region. Such a complicated structure causes some uncertainty for a conventional structure analysis, which leads us to misunderstand the local structure. Therefore we have performed an EXAFS study to obtain the exact local structure and to elucidate the origin of relaxor characteristics from a structural point of view.

Experimental

Ordered and disordered $Pb(In_{1/2}Nb_{1/2})O_3$, hereafter abbreviated as PIN, were examined by EXAFS measurements. The ordered PIN undergoes an antiferroelectric phase transition, whereas the disordered PIN does a diffuse transition that every relaxor experiences. EXAFS spectra for Nb *K*-edge and In *K*-edge were measured at BL10B using a Si(311) channel-cut monochromator, and at BL14A using a Si(551) double crystal monochromator, respectively. Ionization chambers filled with proper gases were employed for detectors, and no focusing mirrors were installed. Low temperature experiments were carried out using a closed-cycle helium gas refrigerator down to 10 K, and high temperature ones were done using a conventional electric heater up to 500 K. Program codes of FEFF7 and UWXAFS3 were employed for EXAFS analyses without any modifications.

Results and discussion

Figure 1 shows the Fourier transforms of k^3-weighted In *K*-edge and Nb *K*-edge EXAFS spectra in the range of k between 3 and 15 $Å^{-1}$ for the ordered and disordered PIN at 10 K. Both Nb and In atoms are coordinated by six oxygen, eight Pb, and six Nb and/or In atoms at respective radial distances of about 2, 3, and 4 Å, as the B-site cation is done in perovskites, ABO_3. The most pronounced feature is profiles of the pair distribution function, abbreviated as PDF, for In-Pb and Nb-Pb around 3 Å. The PDF about Pb atoms is significantly reduced except for In-Pb in the ordered PIN, which reflects the relative displacement of Pb atoms against the BO_6 octahedra.

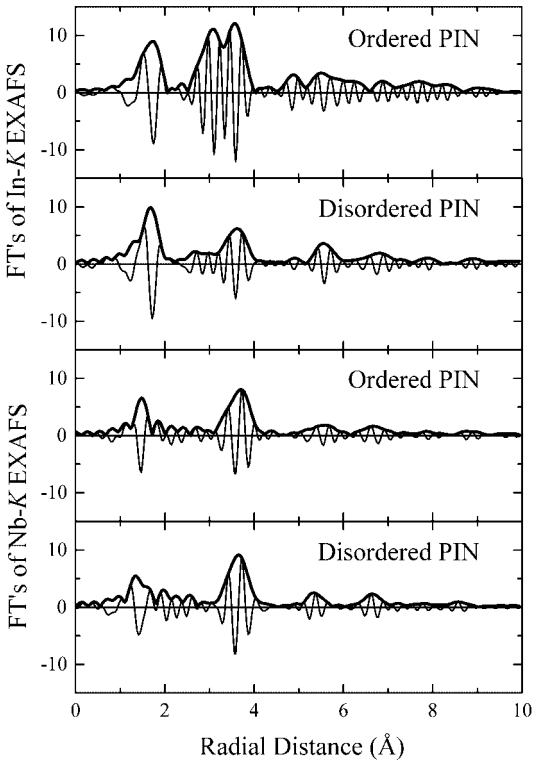

Fig. 1 Fourier transforms of k^3-weighted In *K*-edge and Nb *K*-edge EXAFS for the ordered and disordered PIN at 10 K. Thick and thin curves are absolute and imaginary parts of the Fourier transforms, respectively.

In addition, it should be notice that the magnitude of the PDF for Nb-O around 2 Å is reduced to almost a half of that for In-O in both the ordered and disordered PIN. The fact indicates that an In atom is located at the center of mass of the undistorted InO_6 octahedron, while a Nb atom is displaced resulting in the distorted NbO_6 octahedron. The progressing analysis of the temperature dependency of these local structures will give us further understanding of relaxor characteristics.

References

[1] G. A. Smolenskii et al., Soviet Phys.-Solid State 1, 147 (1958).

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