Local Lattice Distortion Caused by Short-range Charge Ordering in Transition Metal Oxides

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Charge ordering is often observed in transition metal oxides with mixed valence state. It is accompanied with a structural transition because the localized electron has a long range ordering. However, in several materials with the mixed valence and the non-metallic conductivity, the charge ordering is absent, suggesting a short-range charge ordering. We have performed local structural analysis by using atomic pair distribution function (PDF) on such materials to reveal the local lattice distortion caused by the short-range charge ordering.

Cubic spinel compound $LiMn_2O_4$ with the mixed valence of $Mn^{3.5+}$ has non-metallic conductivity [1]. The local structure determined by the PDF analysis has an orthorhombic lattice distortion and includes inequivalent Mn^{3+} and Mn^{4+} sites. It suggests that the valence electron is localized with short-range periodicity, resulting in the non-metallic conductivity in this material [2]. $YBaCo_2O_5$ also exhibits non-metallic conductivity although the Co has the mixed valence of +2.5 above 220K which corresponds with charge ordering temperature [3]. Figure 1 shows PDF observed at 450K. The PDF calculated for the averaged structure shown by gray lines does not reproduce the observed PDF whereas the PDF calculated for the structure model corresponding to the charge ordering state shown by black line reproduces the observed PDF, suggesting the short-range charge ordering above the charge ordering temperature.

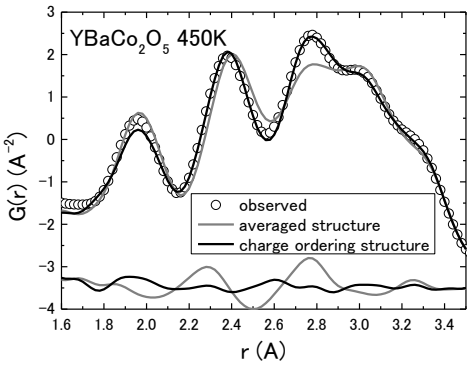

Fig. 1 Observed and calculated PDFs of $YBaCo_2O_5$.

References

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