Local structure of A atom in ABO_3 perovskites studies by RMC/EA-EXAFS

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ABO_3-type perovskite materials are used in numerous technological applications in actuators, electro-optical devices, waveguides, memory cells, solar power convertors, fuel cells, etc. In this study we concentrate on titanates: $BaTiO_3$, $SrTiO_3$, $EuTiO_3$, which exhibit a wide range of low-temperature structural phase transitions [1]. They are extensively studied by all method including x-ray absorption spectroscopy (XAS). Most of the focus is devoted to the TiO_6 octahedra responsible for ferroelectric properties of the material, so, it is no surprise that the most XAS studies are concentrated on Ti K-edge x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS). At the same time, in this study we focus on the local structure of the A atom in ABO_3 perovskites, revisiting old data with new method of analysis.

As a method we will use EXAFS spectra of Sr K-edge for $SrTiO_3$, Ba K-edge for $BaTiO_3$, Eu L3-edge for $EuTiO_3$ obtained in the wide range of temperatures (20 – 400K) analyzed with reverse Monte Carlo combined with evolutionary algorithm method (RMC/EA-EXAFS) [2].

In this study we analyze local structure data for A atom for different structural phases. We compare atom relative positions which include correlations of atomic dynamics with average atomic positions, as well as (MSRD, σ^2) values with (MSD, $\langle u^2 \rangle$) values allowing to assess the size of the correlation effects.

We conclude that A atoms play important role in the properties of ABO_3 perovskites and take active part in phase transitions. The local structure reflecting instantaneous positions of the atoms differs from one expected by diffraction data mainly due to the correlations in the atomic movements.

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