Determination of Atomic Displacements in Perovskite-Type Crystals by Polarized XAFS

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Determination of atomic displacements in perovskite-type compounds is a long standing problem. Accuracy of X-ray diffraction technique in many cases is not sufficient due to strong correlation between temperature and position parameters. Besides there are a lot of evidences that local structure in a number of perovskite crystals differs from the averaged one. Even structure of well known BaTiO$_3$ and KNbO$_3$ crystals is still under discussion since eight site model has been worked out on the basis of the results of diffuse scattering investigation [1]. According to this model Ti and Nb atoms are disordered among several equivalent positions and the phase transitions are of order-disorder type.

We performed polarized XAFS study of Nb positions in KNbO$_3$. The spectra were obtained from a single crystal sample for two orthogonal orientations of the crystal polar axis relative to vector of X-ray polarization. Apparent difference of Fourier transforms of the spectra for these two orientations, presented at Figure as well as results of data fitting indicated that direction of Nb off-center displacement is very close to polar axis direction. Displacement in the orthogonal direction was estimated to be not more than temperature atomic displacements. So it has been shown that eight site model is not valid for KNbO$_3$ and phase transition from the rhombohedral to the orthorhombic phase is essentially of displacive type.

Polarized XAFS technique has been proved to be very powerfull tool for investigation of atomic displacements in perovskite compounds.