Ti K-edge XANES studies of $ATiO_3$ perovskite compounds: comparison between experiment and theory

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$ATiO_3$ (A=Ca, Ba, Sr and Pb) perovskite compounds have been intensively studied mainly due their well-known ferroelectrics properties, which are sensitive to slight variations in lattice distortions and chemical/displacive atomic ordering [1]. X-ray absorption near edge structure (XANES) has been used as a probe of the local atomic structure in order to investigate the mechanism of ferroelectric-paraelectric phase transition for these materials. The pre-edge region of the K-edge XANES spectra of $ATiO_3$ compounds is characterized by a pronounced feature which intensity depends on the degree of distortion around Ti atoms [2,3]. In this study, we present a Ti K-edge XANES spectra of the $ATiO_3$ compounds in which Ti is located in regular or distorted TiO_6 octahedron. We also present *ab initio* XANES calculations made using the high order multiple scattering (MS) code FEFF8.2 [4], which also provides the total and partial electronic density of states (DOS). The calculation gives a semi-quantitative agreement with the experiment and permits the interpretation of XANES in terms of DOS.

Keywords: $ATiO_3$ perovskites, XANES, multiple scattering, DOS.
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[1] M.E. Lines, A.M. Glass, Principles and Applications of Ferroelectrics and Related Materials (Clarendon, Oxford, 1977).
[2] B. Ravel and E.A. Stern, Physica B 208&209, 316 (1995).
[3] R.V. Vedrinskii, V.L. Kraizman, A.A. Novakovich, Ph. V. Demekhin and S.V. Urazhdin, J. Phys. Condens. Matter 10, 9561 (1998).
[4] A.L. Ankudinov and J.J. Rehr, Journal of Synchrotron Radiation 10, 366 (2003).

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