## Ionic Size Induced Defects in Lead Titanate-Zirconate Perovskite Studied by TDPAC Method\*

J. Mestnik Filho, A. W. Carbonari, E. F. Motta<sup>a</sup>, M. Moralles, R. N. Saxena, M. Olzon-Dionysio<sup>a</sup>, and S. D. de Souza<sup>a</sup>

Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP. P.O. Box 11049, 05422-970 São Paulo, SP, Brazil.

<sup>a</sup> Departamento de Física, UFSCar, São Carlos, SP, Brazil

Z. Naturforsch. 53a, 318-322 (1998); received October 31, 1997

Time differential perturbed angular correlation (TDPAC) measurements were carried-out on PbZr<sub>0.8</sub>Ti<sub>0.2</sub>O<sub>3</sub> as a function of temperature. A broad distribution of electric field gradient (EFG) was observed in all cases with a second site for <sup>181</sup>Hf-<sup>181</sup>Ta probes in the R3c phase. The results were analyzed in terms of a model which simulates an attraction of the ions by the smaller Ti ions. The EFG was calculated within the point charge approximation, by averaging over a large number of configurations generated by random distribution of the Ti ions in an ensemble of lattice cells. It was verified that the model reproduces qualitatively the broadening of the TDPAC frequencies as well as explains the second component EFG observed experimentally.

Key words: PbZr<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub>; Perovskites; Crystal Defects; TDPAC Measurements. Reprint requests to J. Mestnik Filho, Fax: +5 51 18 16 - 91 88.