K around the transition temperature. In order to determine precisely the structure at high and low temperatures, Rietveld refinements of a complete 2θ range were performed on the patterns collected below and above the transition temperature either for PLT20 or PLT30. The temperature dependence of the relative dielectric permittivity was also performed. From the final Rietveld refinements it was observed important structural trends and it was possible to determine the range where the ferroelectric-to-paraelectric phase transition takes place. The results observed with the XRD refinements agree with that one observed by electric measurements. Structural details, in terms of short and long-range order, are presented and the correlation between the XRD and XANES/EXAFS data is discussed.

Keywords: Rietveld structural refinement, perovskite structures, phase transitions and structure

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Different models for the polar nanodomain structure of PZN and other relaxor ferroelectrics

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Computer simulations have been carried out to test the recently proposed model [1] for the nano domain structure of relaxor ferroelectrics such as lead zinc niobate (PZN). In this recent model it was supposed that the polar nanodomains are three dimensional, that the observed diffuse rods of scattering originate from the boundaries between domains and that the Pb displacements may be directed along <100>, <111> or <110>. This is in marked contrast to our previously published model [2] which described the polar domains as thin plates with Pb displacements confined to <110> directions within the essentially 2D domains. The present results confirm that <100> and <111> types of Pb displacement are viable possibilities but the number of domain boundaries required to produce sufficiently strong diffuse rods of scattering means that individual domains cannot be described as three dimensional and must still be relatively thin. The current work has been carried out with no direct involvement of the B-site cation ordering that many workers assume is necessary to understand the formation of the polar nanodomains. While it may be true that the B-site cation distribution could provide an underlying perturbation field that might ultimately limit the extent of any polar domain, it is certainly not necessary to produce the observed scattering effects. In an attempt to establish which of the now available models is correct the behaviour of each in an electric field has been explored.

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Keywords: diffuse scattering, relaxor ferroelectrics, PZN

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Structural aspects of the effect of $NaNbO_3$ substitution on quantum paraelectric behavior of $CaTiO_3$

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Several perovskite titanates like $SrTiO_3$, $CaTiO_3$ (CT), $EuTiO_3$, $La_{1/2}Na_{1/2}TiO_3$ and $KTaO_3$ are known to exhibit unusual phenomenon of quantum paraelectricity. For these materials, the dielectric constant increases with decreasing temperature but does not show a peak corresponding to a ferroelectric (FE) or antiferroelectric (AFE) transition. Instead, their dielectric constant becomes temperature independent at very low temperatures. This has been attributed to the suppression of FE/AFE transition due to zero point quantum fluctuations of the lattice. We have recently shown that substitution of Pb^{2+} in CT can stabilise AFE phase with negative Curie-Weiss temperature [1]. In this work, we present evidence for a phase transition at low temperatures in the system $(1-x)CaTiO_3$-$xNaNbO_3$ (CT-xNN), as a result of Na^{+} and Nb^{5+} substitutions at Ca^{2+} and Ti^{4+} sites. $NaNbO_3$ substitution leads to a dielectric anomaly superimposed over a continuously rising paraelectric background of pure CT. This anomaly is characterized by a negative Curie-Weiss temperature indicating an AFE transition. Temperature dependent XRD studies reveal the appearance of weak superlattice reflections below the AFE transition temperature. One of the unit cell parameters of the AFE phase is found to be 6 times that of the paraelectric phase. The paraelectric to AFE transition is shown to be first order as evidenced by a discontinuous change in the unit cell parameters. Our previous study on Pb^{2+} substituted CT [1] and the present study on CT-xNN suggest that CT is an incipient AFE. We also show that the mixed CT-xNN system exhibits morphotropic phase boundary like characteristics [2].

References:

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Keywords: quantum paraelectric, morphotropic phase boundary, antiferroelctric

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Synthesis and characterization of $Bi(Ni_{0.5}Ti_{0.5})O_3$

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Ferroelectric lead zirconate titanate is widely used as integral parts of electrical devices due to the high dielectric and electromechanical properties. However, the toxicity of lead oxide results in serious environmental problems and hence alternative compounds free from lead are urgently under development. Since Bi^{3+} ion has the same electronic structure as the Pb^{2+} ions, Bi-containing perovskites are promising candidates for lead-free ferroelectric ceramics. $Bi(Ni_{0.5}Ti_{0.5})O_3$, BNT, ceramic was

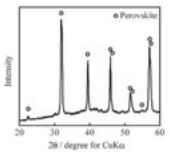

Fig. 1. Powder x-ray diffraction pattern of the BNT ceramic synthesized at 6 GPa, 1000 °C.

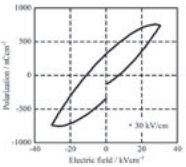

Fig. 2. P-E hysteresis loop of the BNT ceramic.