CRYSTALLOGRAPHY IN MATERIAL SCIENCE

ically, produced by external fields there are 10 types of configurations with non-zero average polarization. It appears that electric field, possibly in combination with mechanical stress, may induce 7 nonequivalent coherent configurations formed each by equivalent domain states with same free energy in the field(s). The form of average tensor properties is given by the corresponding effective symmetry.

By examining tensor properties of the coherent configurations (CC's) we establish five cases where additional relationships between tensor components exist for certain material properties, compared to what is usually obtained for single domain crystals with same macroscopic symmetry. In one case even the stabilizer of each polar tensor of even rank differs from common expectations.

For representative CC's we specify average material tensors up to rank 4 in terms of tensor components of the same selected state.

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Keywords: engineered domain configurations, effective symmetry, average tensor properties

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Lattice Parameters of the PZT 90/10 Ceramic doped with La

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The PZT ceramics have been attracting with considerable attention in a number of different context. One of them are their ferroelectrical properties.

Sample of $Pb_{0.94}La_{0.06}Zr_{0.9}Ti_{0.1}O_3$ was prepared by sol-gel process and sintered at 1200°C for 2 hours.

Investigation lattice parameters of the specimen were studied using X-ray diffraction (XRD). X-ray traces were recorded using a Phillips diffractometer between 20° - 110° (CuK α radiation) with scan step of 0.02° and scan time 14s/step.

In agreement with phase diagram for PLZT system [1] our sample should have a tetragonal structure. To confirm that assumption we prepared two simple simulated scans for tetragonal and rhombohedral structure. On the basis of the results and other data [2] we agreed with that assumption and made preliminary analysis of lattice parameters in profile matching mode. As a results of our investigation we obtained a following parameters: $a=b=4,1051\pm0,0007$ Å, $c=4,1194\pm0,0005$ Å.

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Keywords: ferroelectrics, ceramic materials, powder X-ray diffraction

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Structural Phase Transitions and Hydrogen bonding in $Rb_3H(SO_4)_2$

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Compounds of the type $A_3H(XO_4)_2$, where $A = Li^+$, Na^+ , K^+ , Rb^+ , Cs^+ , $(NH_4)^+$ and X = S, Se are known ferroelectric and paraelectric materials. Recently, structural phase transition in $(NH_4)_3H(SO_4)_2$ have been studied in detail [1]. We have investigated the phase transition in the analogous $Rb_3H(SO_4)_2$, the structure of which at room temperature was determined by Fortier *et al.*[2]. in 1985, at four different temperatures to follow the phase transition behavior. The data were collected on a Bruker Smart Apex CCD system equipped with an

Oxford cryostat at 293K, 100K, 393K and 425K respectively. The hydrogen atom is localized at the midpoint at 100K with respect to the sulfate tetrahedra while at room temperature it is connected with one of the oxygen atoms. DSC studies on a single crystal of the compound indicate phase transitions around 399K and 425K. The crystal structures of $Rb_3H(SO_4)_2$ at four different temperatures show subtle conformational and packing changes and the geometry around the Rb atoms shows different coordination with respect to temperature.

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Keywords: phase transition, hydrogen bonding, coordination

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Relaxor Ferroelectric Behaviour of $Ba_{1-x}A_x(Ti_{0.7}Zr_{0.3})O_3$ Compositions (A=Ca,Sr)

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The relaxor ferroelectric materials exhibit a large range of interesting properties related to their complex order/disorder nanostructures. The relaxor behaviour is well known in lead based compositions. Nevertheless, the latter present a disadvantage due to the toxicity of polluting substances. The actual evolution of research is directed to replace the lead by lead-free compositions [1, 2]. The aim of the present work was to prepare and to characterize some ceramics derived from $BaTiO_3$ by cationic substitution in the 12-C.N crystallographic site.

The various compositions were obtained by solid state synthesis. Room temperature X-ray diffraction analysis allowed us to determine the limits of solid solution. Dielectric measurements exhibit a relaxor behaviour in the range 0 < x < 0.20. Whatever A, Tm decreases as x increases. However, the decrease was comparatively lower in the case of the calcium substitution. This result is related to the size of each cation. For the Ba-Sr substitution the decrease of Tm results from reduction of the c/a ratio. On the contrary, for the Ba-Ca substitution, Ca^{2+} induces a local polar moment leading to a small decrease of Tm. Concerning the strontium substitution, one of the noteworthy characteristic is the very high value in the maximum of ε 'r.

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Keywords: ferroelectric relaxors, lead free materials, disordered materials

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Ferroelectric Phase Transition Mechanism in C₅H₆NBF₄ by X-ray Crystal Analysis

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Pyridinium Tetrafluoroborate $C_5H_6NBF_4$ (abbreviated to PyBF₄) undergoes a ferroelectric-paraelectric phase transition at T_1 =238.7K, and another phase transition at T_2 =204K [1, 3]. From the NMR studies [2], the pyridinium and tetrafluoroborate ions were the dynamical disorder state at room temperature. It was suggested that the ordering of these ions was linked to the successive phase transitions. From the X-ray diffraction study [3], the disorder state of the pyridinium and tetrafluoroborate ions was also reported. However, a report of the crystal structure analysis at low temperature was not found. The crystal structure analyses at low temperature phases in PyBF₄ were very important in order to clarify the mechanism of the successive phase transition in this material.

Re-investigation of the single-crystal X-ray structure analysis in