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Local-site cation ordering of Ln3+ ions in doped PbTiO3

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The study of doped PbTiO3 with lanthanide (Ln3+) elements is an alternative way in order to obtain high density samples with near optimal piezoelectric properties, avoiding at the same time a high porosity microstructure and a crystal structure with a large c/a ratio. X-ray diffraction (XRD), extended X-ray absorption fine structure (EXAFS), and scanning electron microscopy experiments were carried out in the (Pb0.88Ln0.08)TiO3 ferroelectric system with a perovskite type structure (Ln = La, Sm; Eu, Gd and Dy). Qualitative EXAFS analysis has shown that Ln ions substitute to Pb2+ and Ti4+ ions at A and B sites of the ABO3 structure, respectively except for La doped PbTiO3. The XRD pattern refinement was consistent with the Ln ion substitution at both A and B sites, which provides the formation of donor and acceptor type defects. The shape of the observed X-ray lines profiles has shown features, which are known for this kind of ferroelectric material to be typical of the ferroelectric domains microstructure. A phenomenological model has been used for fitting the diffraction profiles by the Rietveld method [1]. A two phase model considering isotropic size and anisotropic strain broadening was used as a suitable approximation for describing the peculiar peak shapes of the diffraction pattern[2], resulting in a useful approach for analyzing the effects of the domains microstructure. As example, the figure 1 shows the result of the XRD pattern refinement for the sample (Pb0.88Eu0.08)TiO3 taking into account asymmetric and anisotropic effects [3]. The observed and calculated patterns are denoted with dots and continuous lines, respectively. Bragg reflections are represented by vertical marks. The difference between the observed and the calculated data is plotted at the bottom.

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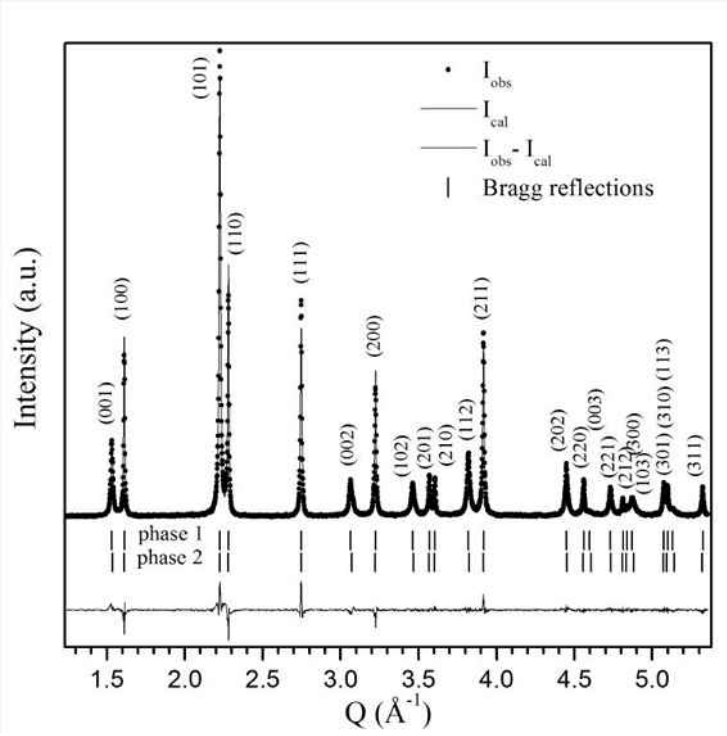

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