Nanocomposites and nanomaterials

Distinguishing characteristics of phase transitions in $KTa_{1-x}Nb_xO_3$ nanoparticles

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Solid solutions of $KTa_{1-x}Nb_xO_3$ (KTN) are alternative materials to replace lead-containing materials. Studies of the newly fabricated samples are primarily aimed at the detection of size effects, in particular, at the features which are appeared in the region of the phase transition.

A careful study of the spectroscopic characteristics of the transverse optical modes of the Raman spectra has been carried out within the temperature range, which contains all phase transitions that occur in these compounds [1,2]. It was found that the phase transition temperature in nanosized powders is shifted with respect to temperature observed in corresponding macrocrystals. In addition, on the samples of $KTa_{0.5}Nb_{0.5}O_3$ we registered the signs of a new structural transformation near -100^0C. To explain the established features of structural transitions and new phase states in nanocrystals of $KTa_{1-x}Nb_xO_3$ system we propose a theoretical model that takes into account the local lattice deformations, arising from the increased concentration of defects near the surface of the particle [3]. We also conduct a quantitative comparison between theoretical and experimental results. It is unexpectedly revealed that the dependence of T_c on the Nb content x becomes nonmonotonic at $R < 20$ nm. For compressed particles ($\eta < 0$) T_C increases with the radius decrease. For stretched particles ($\eta > 0$) situation is the opposite. Thus, from the comparison of theory with experiment, a crucial contribution of Vegard strains in the external size effect in ferroelectric nanoparticles is established.

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