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INVESTIGATION OF LINE SHAPE OF ESR SPECTRA IN $BaTiO_3$ NANOPOWDERS

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ESR spectra were recorded in the powder samples of $BaTiO_3$ fabricated by rate-controlled synthesis. The average sizes of the particles of the samples were 34.7 nm; 48.0 nm; 59.0 nm; 85.8 nm and 97.9 nm. ESR measurements were recorded at room temperature with a spectrometer operated at 9.4 GHz. We observed Fe^{3+} (S = 5/2) ESR spectrum which was described by tetragonal symmetry spin-hamiltonian. The position of the most intensive line that corresponds to $\pm 1/2 \leftrightarrow \mp 1/2$ transition was characterized by effective g-factor in vicinity $g_{eff} \cong 2$. The line shape and intensity appeared to be strongly dependent on the particles size. In particular the decrease of the intensity and broadening of the line was observed with the decrease of the particle size. The characteristic feature of the line shape was its asymmetry that increased with the decrease of the size of nanoparticles. The later fact gives evidence that the observed line is a superposition of at least two independent lines. The computer stimulation made it possible to extract these two lines, the ratio of their integral intensity being dependent on the particle size. This fact and small difference ($\sim 10^{-3}$) between g-factors of the lines speak in favor of statement that the line with smaller g-factor originated from the region that "feels" the influence of the particle surface. The position of another line corresponds to Fe^{3+} ion in the bulk $BaTiO_3$.

The theory of ESR spectra of nanosize powder samples is proposed. The consideration was performed in core and shell model which are respectively the nanoparticle regions unperturbed and perturbed by the surface influence. The shift of resonance frequency by surface tension was taken into account. The splitting of spectra into two lines with particle size decrease which like those in the bulk and on the surface was shown to be characteristic feature of nanomaterials spectra. Detailed comparison of the theory with experiment had shown that it fitted pretty good the observed peculiarities of $BaTiO_3$ ESR spectra.