

Crystal lattice dynamics of the substituted solid solutions in the Bi(Gd)-Fe-O and Bi(Nd)-Fe-O systems

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The bismuth ferrite BiFeO₃ is promising as magnetoelectric material because both the ferroelectric and antiferromagnetic orders coexist in this material at room temperature. Doping of BiFeO₃ or the substitution of bismuth by other chemical elements can modify its physical properties. The goal of this paper is to determine the influence of the bismuth substitution by gadolinium and neodymium on crystal lattice dynamics at room temperature.

The substituted solid solutions of BiFeO₃ of the types Bi_{1-x}Gd_xFeO₃ and Bi_{1-x}Nd_xFeO₃ with the atomic part of the substitutive element x up to 0.20 were synthesized by means of the solid-state reaction method using powders of oxides Bi₂O₃, Nd₂O₃, Gd₂O₃, and Fe₂O₃ of pure grade quality. The X-ray diffraction method was applied using the diffractometer Dron-3 on Cu K α radiation. The experimental data were collected during scanning repeated ten times in the 2Θ range from 20° to 90° at the scanning speed of 10°/6 min. The infrared reflection spectra of the samples in tablet powder mixtures were recorded with VERTEX 80v FT-IR spectrometer (Bruker). As standards for the recording of the absolute values of the reflection coefficient R , an aluminum mirror with $R = 97\%$ and a single crystal silicon wafer were used.

The X-ray patterns show the displacement of the positions of reflexes of BiFeO₃ with the substitution of bismuth by gadolinium and neodymium. This confirms the formation of the solid solutions Bi_{1-x}Gd_xFeO₃ and Bi_{1-x}Nd_xFeO₃. The lattice constants of the formed solid solutions decrease with the increase of the content of the substitutive element Gd. This may be explained by the lower ionic radii of Gd³⁺ with respect to Bi³⁺. The small inclusion of the impurity phases of Bi₂₅FeO₃₉ and Bi₂Fe₄O₉ in addition to the main phase of BiFeO₃ is also indicated. Nevertheless the small presence of the impurity phases allows to make conclusions regarding physical properties of these materials, including their crystal lattice dynamics.

Two extremums at 18.2 μm (strong extremum) and 22.5 μm (rather weak extremum) on the infrared reflection spectra of the solid solutions Bi_{1-x}Gd_xFeO₃ and Bi_{1-x}Nd_xFeO₃ were discovered. The extremum at 18.2 μm is caused by the bending of the mechanical vibrations of the Fe – O bonds and the extremum at 22.5 μm is caused by the stretching of the mechanical vibrations of the Fe – O bonds. The increase of the atomic part of the substitutive element x up to 0.20 leads to the growth of the reflectivity and the absorption coefficients of the solid solutions Bi_{1-x}Gd_xFeO₃ and Bi_{1-x}Nd_xFeO₃ in comparison with BiFeO₃. The displacement of the absorption band maximum into the side of the spectrum with longer wavelengths with the increase of the content of the substitutive elements was also found. Such behavior of the spectra can be explained by decreasing elastic constants of the solid solutions Bi_{1-x}Gd_xFeO₃ and Bi_{1-x}Nd_xFeO₃ occurring when the new substitution-induced bonds Gd – O and Nd – O are formed.