

The spatial distribution of copper ions incorporated into LiNbO₃ crystal during high temperature annealing

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The incorporation of copper ions into lithium niobate (LN) during high-temperature annealing was studied. The samples of LN (7(X)×15(Y)×32(Z) mm) used in the experiments were cut from the optical quality congruent crystals produced at SRC "Carat" and annealed additively in air at 1073 K for 3h+6h+12h. The samples were covered by CuO powder during annealing. After each stage they were cooled and their transmission spectra were registered in Z direction. Absorption spectra of annealed LN samples were registered by UV3600 Shimadzu spectrophotometer in the 300...800 nm spectral range. After the last stage of annealing the samples were cut on wafers (1 mm in thickness) used for registration of the optical absorption in different crystallographic directions and in different depths into the samples. The specially designed device allowed scanning of the light beam with the step of 20 μm.

In the spectra of annealed samples (light propagated in direction of diffusion) we observe shift of the absorption edge to higher wavelength region and appearance of a weak broad band with a maximum near 1000 nm. The shift of the edge and the magnitude of absorption near 1000 nm increase with duration of annealing that agrees with the results of [1]. In spectra of additional absorption the band with the maximum near 400 nm is also observed. Obviously, the observed changes of the optical spectra were caused by Cu⁺ and Cu²⁺ ions incorporation into the crystal. These changes can be explained under the assumption that copper is partially kept in the form of nanoparticles of CuO in the area close to the sample surface. The presence of nano-inclusions is confirmed by XRD studies of the surfaces of the annealed samples. The incorporated ions were spatially separated on two regions. One of them corresponds to copper ions in the state of 2+ and the other one – to copper in the monovalent state. The final conclusions about the mechanisms of copper diffusion in LN crystals require additional research.

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