NMR ANALYSIS OF Mg ION LOCALIZATION IN $LiNbO_3$ CRYSTAL

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Lithium niobate (LN) crystals doped with Mg or Zn are the objects of particular interest and extensive investigations because it was found that these dopants are responsible for increasing of resistance of LN to optical damage. Till now there are essential divergences in a questions on localization of Mg^{2+} ions in LN crystals, which have been grown up from the congruent melt with addition of MgO and an mechanisms of charge compensation of incorporation of Mg^{2+} ions in LN structure.

Let us believe, that the general chemical formula of LN:Mg crystal can be written as: $Li_xMg_yNb_zO_3$. Under condition of 100 % filling of niobium structural positions, all known models of localization of Mg^{2+} ions in LN structure can be presented by following structural formulas:

$[Li_xMg_yNb_{z-1}\square_{2-x-y-z}]NbO_3$ for $z > 1$
$[Li_xMg_{y+z-1}\square_{2-x-y-z}][Nb_zMg_{1-z}]O_3$ for $z < 1$

On the basis of the analysis of the known experimental data about dependence of Li/Nb ratio (*R*) in the LN crystal on the MgO content [1-3] it has been established that the quantity of Mg_{Li} ions monotonously grows with increasing of MgO content; and, when the MgO content is above threshold value, Mg ions replace as ions Li_{Li} and Nb_{Nb}. These conclusions are in good agreement with the model offered in [4].

Series of $LiNbO_3$ crystals with various Mg contents was investigated by nuclear magnetic resonance (NMR) of ^7Li and ^{93}Nb. It is shown, that under MgO content above threshold, the additional ^{93}Nb NMR line, which corresponds to the nuclei of Nb_{Li} ions, disappears. According to our data, under increasing of the Mg content in the crystal, the fast growth of the width of the central line of ^{93}Nb NMR spectra is observed. It indicates the growth of volume concentration of replacement type defects.

References

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