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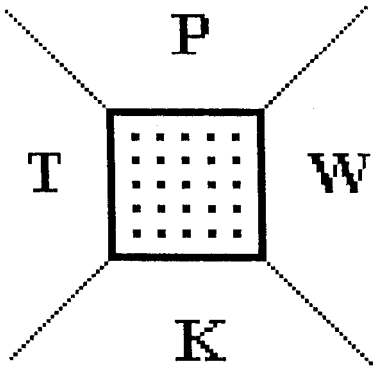

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NMR STUDY OF INTRINSIC DEFECTS INTO CONGRUENT LITHIUM NIOBATE

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The computer simulations of Nuclear Magnetic Resonance (NMR) spectra of ^{7}Li and ^{93}Nb nuclei for different models of the intrinsic defects in single crystal of congruent lithium niobate (LN) have been performed. The simulations of the NMR spectra have been performed assuming that the distortions of lattice introduced by the intrinsic defects are negligible and the defects are distributed randomly in crystal lattice of LN.
The analysis of the simulated and experimental NMR spectra of ^{7}Li nuclei show that the shapes of the resonance lines are not sensitive to the type of the intrinsic defects and the observed additional quadrupolar lines of ^{7}Li in LN [1-3] are not due to the intrinsic defects. The calculations of the potential relief for Li ion into distorted LiO_6 octahedron are showing that the potential function has four minima: 1) three equivalent minima U_1 shifted from c-axis and related by symmetry axis 3 and 2) one minimum U_2 sited on c-axis. From calculations follows that $U_1<U_2$. In order to explain the additional quadrupolar lines of ^{7}Li we assumed that the basic lines in NMR spectra of ^{7}Li nuclei may be related with those lithium nuclei which occupy the three minima U_1 and undergo the fast reorientation about its threefold axis. Than weak quadrupolar lines are related with the Li ions which occupy the potential minimum U_2. The simulated NMR spectra of ^{7}Li nuclei according to this model are in good agreement with experimental one.
The analysis of the simulated and experimental NMR spectra of ^{93}Nb nuclei show that the Nb-site vacancy model is not consistent with the NMR data and only Li-site vacancy model may be considered as the proper intrinsic defect model of the LN structure. From our results it follows that the most probable defects into $LiNbO_3$ are complex [Nb + $3V_{Li}$] and isolated vacancies V_{Li} of lithium ions [2,4-6]. The observed additional NMR lines of ^{93}Nb nuclei at some orientations of LN crystal into external magnetic field support this model of the intrinsic defects into congruent lithium niobate.

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