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ABSTRACTS

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EP – 7/6 THE PECULIARITIES OF THE STOICHIOMETRIC LiNbO₃ CRYSTALS STRUCTURE IN THE PARAELECTRIC PHASE

Sergeev N.A.¹, Shostak R.I.², Yatsenko A.V.²

¹ *University of Szczecin, Szczecin 70-451, Poland;*

² *Taurida National University, Simferopol 95007, Ukraine.*

The computer simulation of the LiNbO₃ structure in a high-temperature paraelectric phase ($T > 1460$ K) was carried out. It is well-known, that during the phase transition into the high-temperature phase, Nb⁵⁺ moves into the centrosymmetric position within NbO₆ octahedron [1]. But for Li⁺ two models were proposed in the literature. The first model is the classical displacive model – Li⁺ moves into a triangularly coordinated site within the oxygen layer [1]. The second model is order-disorder model – the Li⁺ ions are randomly distributed on both sides of this oxygen plane [2]. This model was proposed to explain a neutron scattering experimental data. It is need to note, that according to this model, the displacement of the Li⁺ ions in z-direction (polar axis) relative to the oxygen layer Δz is extremely large: $\Delta z = \pm 0.50 \text{ \AA}$.

The classical electrostatic methods of calculation were used for the computer simulation of the LiNbO₃ structure. The analysis of the stoichiometric LiNbO₃ structure in the paraelectric phase is showed that (Nb – O) bonds probably are ionic bonds, so the effective charges of the Nb⁵⁺ and O²⁻ ions are close to the their formal charges. It was been shown earlier [3] that the anisotropy of the electronic polarizability of O²⁻ is the consequence of the overlapping of the outer electronic shells of the Nb⁵⁺ and O²⁻ ions, so the electronic polarizability of the O²⁻ ions in the paraelectric phase must be isotropic. By using of this basic postulates it was computed the electrostatic potential relief for the nearest neighbourhood (0.6 Å) of the triangularly coordinated site within the oxygen layer (Li⁺ position according to [1]). It was believed that the structure of the crystal is close to the first model. Only pure ionic and electric dipole contributions to the electrostatic potential were taken into account. The repulsive interaction potential relief calculations for the Li⁺ ions was carried out too. The Bohr – Mayer approach was used for this calculations, and the parameters of the short - range potential were equal to estimated in [4]. In the same manner it was analyzed the potential relief for the nearest neighbourhood of the Li⁺ site for the order – disorder model. The Li⁺ site displacements Δz were randomly distributed for the Li⁺ sites into the sphere with radius $R = 60 \text{ \AA}$, and the some random realizations of the static crystal structure were analyzed.

The analysis of the potential relief shows, that the static structure with the random displacements of the Li⁺ ions is not satisfy to the stability of the crystal structure and the static Li⁺ ions displacement leads to the sufficient distortions of the O²⁻ and Nb⁵⁺ sublattices. On the other hand the potential relief for the nearest neighbourhood of the Li⁺ site computed according to the first model is the such, that the Li⁺ ion due to the high mobility can be displaced along z axis of the crystal at $|\Delta z| < 0.5 \text{ \AA}$. So the peculiarity of the LiNbO₃ structure in the paraelectric phase is the fast dynamic displacement of the Li⁺ ions at the equal probability on the both sides of the oxygen plane below the former Li⁺ site in ferroelectric phase.

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