

Structural investigation of Lithium Niobate between 293 and 100 K

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Abstract

A comparative study have been carried using X-ray diffraction investigation on a single crystal of LiNbO₃ at 120 K and ambient temperature. The Lithium Niobate (LiNbO₃) is a ferroelectric inorganic compound largely used in the integrated and guided optical waves.

The LiNbO₃ compound is a also known for its interesting properties in the in the non-linear optical field. The components of the first hyperpolarizabilty present large values compared to the known inorganic compounds in the non linear optical domain. The according field transparency extends from 350 to 5000 nm and its manufacturing process is well controlled.

The experimental data were obtained from high resolution x-ray diffraction experiment. The data processing was carried using the formalism as described by Belessing in 1989. The structure refinement was carried out using the program MOLLY taking into account the contribution of the non spherical electron distribution. The reliability factors obtained at the end of the refinement are 6 % for ambient experiment and about 3 % for the low temperature investigation.

This present investigation has shown clearly a small displacements of 1 % (figure-1) of the Oxygen atoms around the Li-Nb axis. However, the crystal structure of Lithium Niobate seems to be stable in the large temperature investigated domain.