

MASTER'S THESIS

FTIR and XPS of congruent and stoichiometric LiNbO₃

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FTIR and XPS of Congruent and Stoichiometric LiNbO₃

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Abstract

We have studied defect structures of various kinds of (LiNbO₃) LN single crystals. Stoichiometric LN (SLN) and congruent LN (CLN) as well as Er-doped and Mg-doped LN were examined. With the use of Fourier Transform Infrared spectroscopy, their O-H bond-stretching vibration peaks, transition peaks and polarization characteristics were measured. Also investigated was the X-ray photoelectron spectra (XPS) of these samples.

The absorption bands due to OH band-stretching vibrations in stoichiometric LN crystals locate at 3465.5 cm⁻¹ with a half-width of 2.9 cm⁻¹. This narrow band indicates that there are specific lattice sites for the hydroxyl defects. For congruent LN, we have resolved three more peaks on the higher-energy side, at 3481.3, 3489.6 and 3499.3 cm⁻¹ respectively. The results indicate that stoichiometric LN possesses a more perfect lattice structure than a congruent one. Appearance of these higher energy transitions is the consequence of the defects due to the Li deficiency in the crystal. It has been clarified that the behavior of $\nu(\text{OH})$ reflects the defect structures. Therefore, infrared absorption spectroscopy can serve to characterize the Li deficiency in LN to high accuracy. On the basis of the polarization characteristics, its result indicates that the angle between the direction of the O-H bonds and the plane perpendicular to the c-axis, where Mg ions are doped, matches with the angle between the direction of Li-O bonds and the 336 pm oxygen plane. The behavior of $\nu(\text{OH})$ supports the Li-site vacancy as the defect structure model.

Core level XPS spectra of crystalline LN samples have also been measured. [Li], [Nb] and [O] concentrations were calculated from their corresponding XPS peak areas, as well as the ratios of [Li]/[Nb] on the surfaces determined. By studying the chemical shift of photoelectron lines, the Li 1s, Nb 3d spectrum indicated +1 valence and +5 valence of Li and Nb respectively. Its result indicates that the material properties difference between SLN and CLN is mainly due to the defect structures.

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