OH^- Absorption of Zn-Doped $LiNbO_3$ Single Crystals after Proton Exchange

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An investigation of the OH^- absorption spectra of Zn-doped $LiNbO_3$ single crystals with doping concentrations from 0.0 to 8.3 mol% after proton exchange (PE) is carried out. Before PE treatment, the absorption bands are found centered at approximately 3485 cm^{-1} for the samples with Zn-doping concentrations below 7.5 mol%, whereas two distinct bands at 3505 and 3530 cm^{-1} are clearly observed for the samples with Zn-doping concentrations above 7.5 mol%. After PE treatment, an absorption band at 3505 cm^{-1} is predominant for all the samples, and this is attributed to the high concentration of H^+ ions substituting Li atoms. A theoretical investigation using the hybrid density functional B3LYP method with a simple cluster structure shows that the origins of the 3485 and 3530 cm^{-1} absorption modes correspond to the Li- and Nb-vacancy models, respectively.

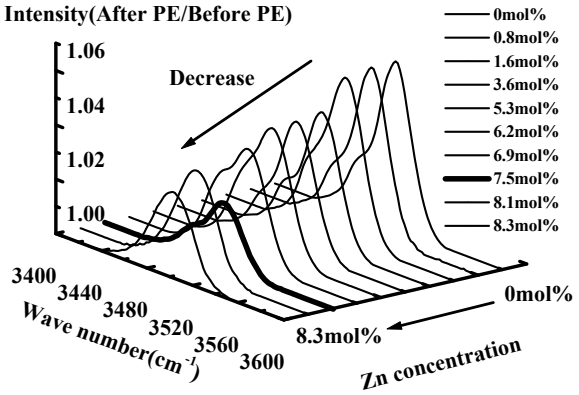

Figure 1. OH^- absorption spectra of Zn-doped $LiNbO_3$ with Zn-doping concentrations from 0 to 8.3 mol% after PE treatment.

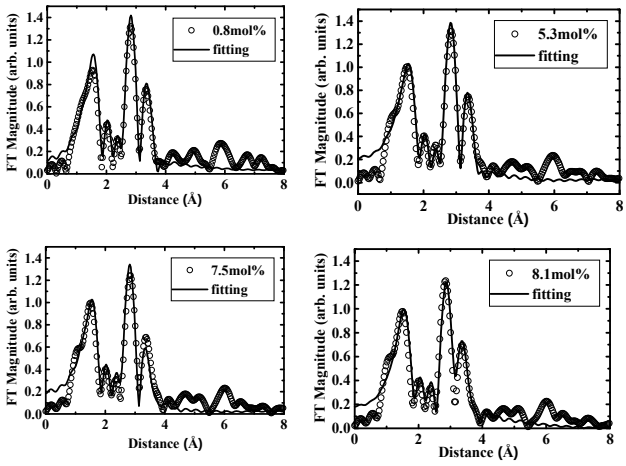

Figure 2. Zn-core EXAFS absorption spectra with fitting

In summary, we studied the proton-exchange OH^- absorption spectra of Zn-doped $LiNbO_3$ single crystals. Below 7.5 mol% Zn-doping concentration, the after-PE-treatment samples show similar absorption bands, which are 3467, 3485, and 3505 cm^{-1}. For the samples with Zn doping concentrations above 7.5 mol%, only the 3505 cm^{-1} band is found for the after-PE-treatment samples. Also, the lineshape and intensity of the 3530 cm^{-1} band are not affected by PE, and this implies that the 3530 cm^{-1} band cannot be formed by PE. This is totally different from the samples with a doping concentration below 7.5 mol%. On the basis of our theoretical investigation, this is mainly due to the Nb vacancy surrounded by Zn_{Li}^+ ions.

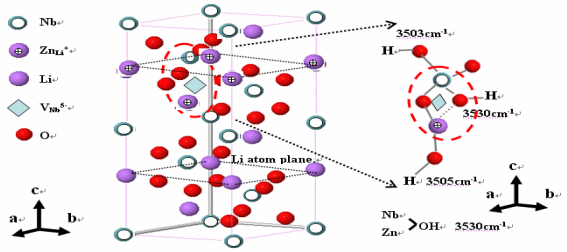

Figure 3. Nb-vacancy model