Crystal structure variation of rare earth-doped $LiNbO_3$ during milling

G, Dravecz[1]*, L. Péter[1], T. Kolonits[2,3], K. Lengyel[1]
*lead presenter: dravecz.gabriella@wigner.hu
1 Wigner Research Centre for Physics, Budapest, Hungary
2 Institute for Technical Physics and Materials Science, Centre for Energy Research, Eötvös Loránd Research Network, Konkoly-Thege Miklós út 29-33, H-1121 Budapest, Hungary
3 Department of Materials Physics, ELTE Eötvös Loránd University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary

Lithium niobate ($LiNbO_3$) optical single crystal doped with different rare earth (RE) ions plays important roles for coherent quantum optical experiments (electromagnetically induced transparency, slowdown of light pulses, coherent quantum memory)[1]. The expansion of applications is increasingly requiring the production of RE-doped $LiNbO_3$ particles in the nanoscale region. In these crystals, the RE ions can act like single photon source, which can be the bases of a coding system of the quantum computer providing complete inaccessibility to strangers.

Yb- and Er-doped $LiNbO_3$ nanocrystals were prepared by high-energy ball milling of stoichiometric $LiNbO_3$ bulk single crystals (doped with Yb or Er) with a Fritsch Pulverisette 7 Premium line planetary mill. The milling parameters were described in a previous article[2]. By changing the ball size and the milling time, a series of samples was made with the particle diameters varying from 300 nm to 10 nm. The size and shape of the nanocrystals were followed by Dynamic Light Scattering and Scanning Electron Microscope measurements, respectively. Emerging phases were assigned by X-ray diffractometry with a Rigaku Smartlab diffractometer. The absorption spectra of RE ions were recorded by a BRUKER IFS 66/v instrument.

Structural change of the $LiNbO_3$ lattice caused by the milling process can be observed with the investigation of the absorption properties of the RE dopant. Two characteristic peaks were found in the Yb spectra (10200 cm^{-1} corresponds to a crystalline structure and 10240 cm^{-1} corresponds to an Nb-rich amorphous structure). With a decrease of the particle size, an increasing ratio of the band intensities of the amorphous and crystalline structures was observed. The peak corresponding to the crystalline phase completely disappeared in the samples with diameter at about 10 nm. A similar phenomenon was found during the milling process of the Er-doped $LiNbO_3$. While the 300 nm fraction still showed well-separated Er peaks characteristic of the crystalline nature of the sample, the Er absorption band related to the amorphous structure was found only when the particle size reached 10 nm.

With regards of the use of the RE-doped nanoparticles as single photon sources, the exact knowledge of the structure of their immediate environment is essential. This research helps to understand the structural changes of the RE-doped $LiNbO_3$ bulk crystals during the grinding process.

References

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