

1 08 01 324 Experiment report

From the study of the L_{III} -Erbium edge (8360 eV) the local environment of the Er atoms was studied for some Er bulk LiNbO_3 crystals and on Periodically Poled Lithium Niobate (PPLN) $\text{Er}:\text{LiNbO}_3$ crystals. The samples were prepared by varying both the composition of the starting material and the growth conditions (pulling and rotational rates).

In Figure 1 we report the EXAFS $\chi(k)$ signal, respectively, for $\text{Er}:\text{LiNbO}_3$ crystals doped with different Er content (0.5 and 2 mol.) and for PPLN $\text{Er}:\text{LiNbO}_3$ doped with 0.2 mol. of erbium. In Figures 2 and 3 the results of the Fourier transform of the EXAFS spectra are reported as a function of the interatomic distance R (dotted points) fitted within the first 3 shells (continuous line). In table 1 we summarize the interatomic distances of Er-O (first shell), Er-Nb (second shell), Er-Nb (third shell) resulting from fitting procedures.

From EXAFS measurements it clearly emerges that the best fitting procedure requires the contribution of one oxygen shell and two Nb shells around the Erbium atom. The interatomic distance of the second shell ranges between 2.99-3.05 Å depending on the Er content in the material. This value is compatible within the experimental error with the Li-Nb distance (3.06 Å) in pure LiNbO_3 crystals. Moreover, the coordination distance of the third Er-Nb shell ranges between 3.26-3.29 Å. These results indicate that Er cannot occupy the Nb site otherwise the 2nd shell Er-Nb distance should be close to 3.76 Å. They suggest, instead, that Er lies in the Li site. The differences in the bonds length of the third shell are due to the different atomic radius of Er (0.96 Å) with respect to Li (0.60 Å).

As in LiNbO_3 crystals the Li and Nb atoms are surrounded by oxygens in distorted octahedral configuration, different Li-O and Nb-O interatomic distances are present. It is common to assume a not distorted octahedron, i.e. only one Li-O (Nb-O) distance value. Under this assumption, the mean value of Li-O distances in pure LiNbO_3 is close to 2.15 Å while for Nb-O bonds it is close to 2.00 Å: in the analyzed $\text{Er}:\text{LiNbO}_3$ samples the Er-O distance is between 2.17-2.22 Å and near the Li-O value. This further confirms the assumption that Er atoms lie in the Li sites.

Sample	$R(\text{Å})$		
	Er - O	Er - Nb	Er - Nb
Bulk 0.5 mol. %	2.17 ± 0.04	3.05 ± 0.09	3.29 ± 0.04
Bulk 2 mol. %	2.22 ± 0.04	2.99 ± 0.08	3.26 ± 0.02
PPLN 0.2 mol. %	2.17 ± 0.02	2.97 ± 0.07	3.26 ± 0.04

Table 1: Interatomic distances R of the Er-O, Er-Nb bonds in some erbium bulk doped LiNbO_3 crystals.

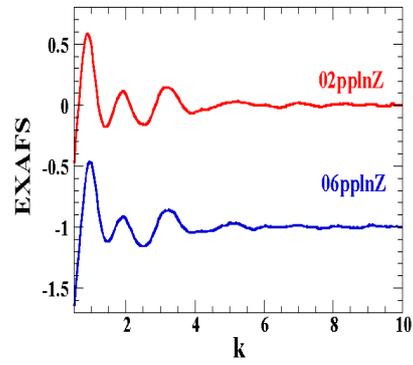


Figure 1: The EXAFS spectra for the Er:LiNbO₃ PPLN samples.

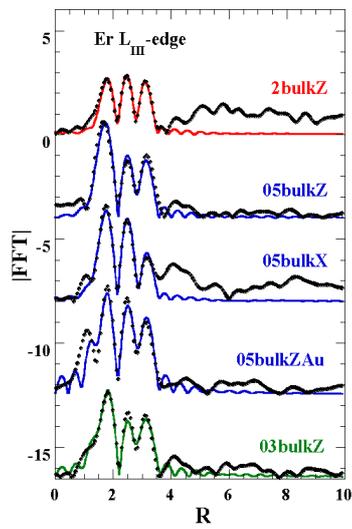


Figure 2: The Fourier Transform of EXAFS spectra for the Er:LiNbO₃ bulk samples.

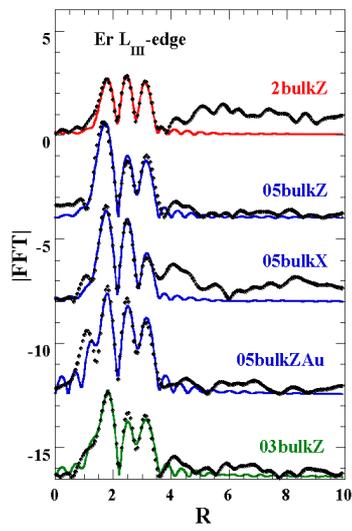


Figure 3: The Fourier Transform of EXAFS spectra for the PPLN Er:LiNbO₃ samples.