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Supporting information

Role of heat treatment on the structural and luminescence properties of Yb^{3+}/Ln^{3+} (Ln = Tm, Ho and Er) co-doped LaF_3 nanoparticles

Patricia Y. Poma, [a*] Tasso O. Sales, [a*] kagola U. Kumar [b] and Carlos Jacinto [a, †]

[a.] *Group of Nano-Photonics and Imaging, Instituto de Física, Universidade Federal de Alagoas, 57072-900, Maceió, Alagoas, Brazil.*
[b.] *Department of Physics, School of Physical Sciences, REVA University, Bengaluru-560 064, Karnataka, India*

** These authors contributed equally to this work*
† Corresponding author: cjacinto@fis.ufal.br

The XRD data for samples without heat treatment (RT) and thermal treated at 300, 500, 700, and 900 °C were analyzed with the Rietveld profile refinement method [1] by using the GSAS-II - Crystallography Data Analysis Software. The Rietveld method is based on minimizing the residual S equal to the sum of the square of the difference between the observed and calculated intensity for every data point in the diffraction pattern. The unit cell, atomic position, Gaussian profile form, and background parameters were all refined but not always simultaneously. The least-squares calculations were carried out until a constant R_{wp} value was obtained in the refinement between the entire observed and calculated powder diffraction pattern [2, 3].

Table 1 summarizes the results of the refinement by the Rietveld method for LaF_3:10Yb/2Ho NPs without (RT) and heat treated at 300, 500, 700 and 900 °C. The X-ray diffractograms calculated and observed, as well as the difference between the profiles are shown in Figure 1, where we have the samples RT and also those treated thermally. In the heat-treated sample at 500 °C, it is noted that both the observed and calculated peaks are very similar, better representing the structure of LaF_3 in the hexagonal phase. For the sample treated at 700 °C, a weight percentages of 80.0%, 5.5% and 14.5% were obtained for the hexagonal LaF_3, tetragonal LaOF and rhombohedral LaOF phases, respectively. Finally, for the sample treated at 900 °C, only the tetragonal LaOF phase is observed. The deviations between the observed and calculated powder diffraction patterns are probably associated with the

significant overlap of the Bragg reflections in the spectra. Some discrepancies may be also due to the preferred orientation effect of the structures [4]. The R_{wp} and S values obtained during the refinement were well satisfactory for the studied system.

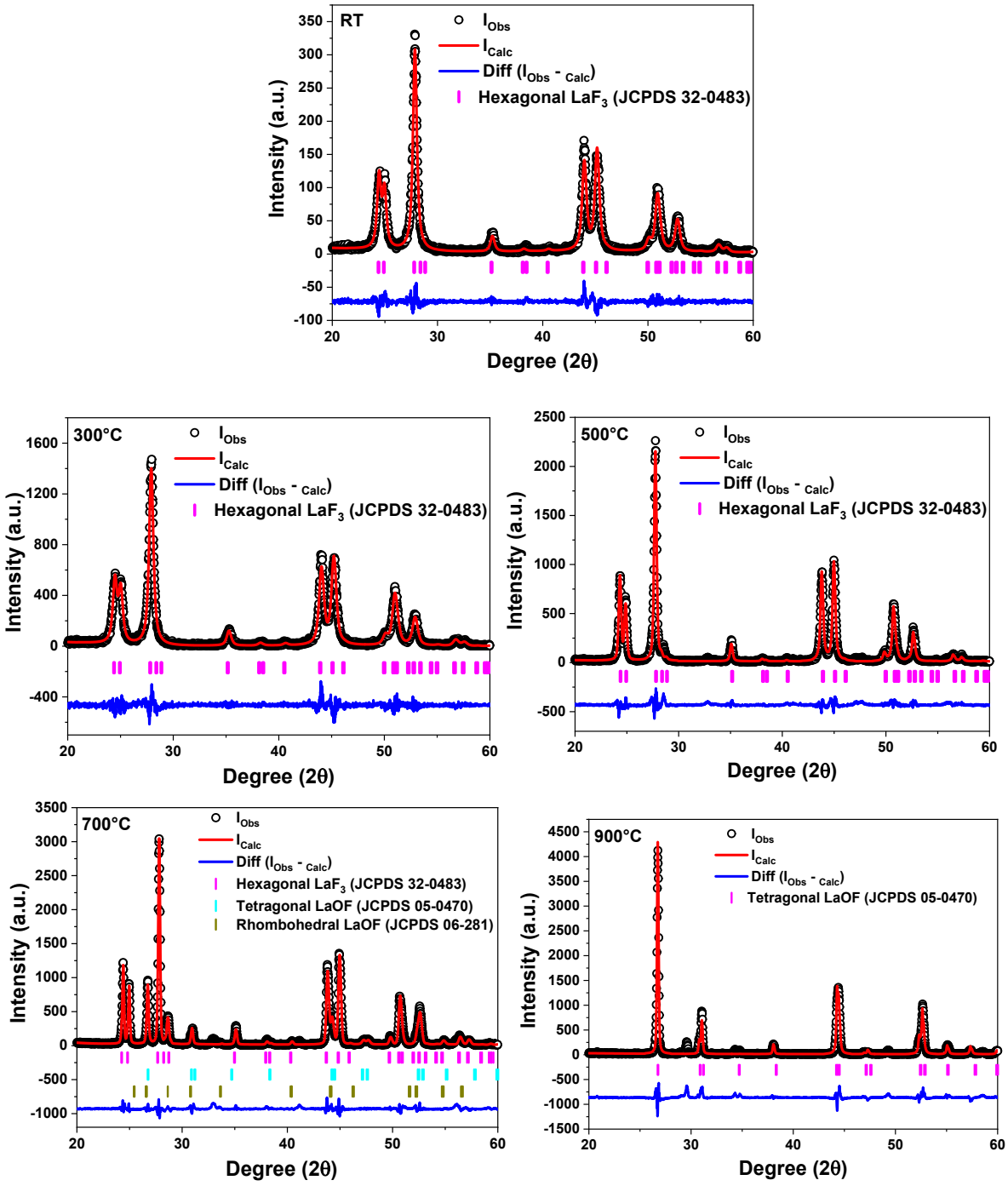

Figure 1: X-ray diffractograms for LaF_3:10Yb/2Ho without (RT) and heat-treated samples at 300, 500, 700, and 900°C.

Table 1: Refinement results for LaF_3:10Yb/2Ho without (RT) and heat-treated samples. R_p is the statistically expected value for the weighted profile (R_{wp}). S is the confidence factor of refinement.

Temperature (°C)	**RT**	**300**	**500**	**700**			**900**
Space group	$P\bar{3}c1$	$P\bar{3}c1$	$P\bar{3}c1$	$P\bar{3}c1$	P4/nmm	$R\bar{3}m$	P4/nmm
Structural symmetry	Hexagonal	Hexagonal	Hexagonal	Hexagonal (80.0%)	Tetragonal (5.5%)	rhombohedral (14.5%)	Tetragonal
Network parameters (Å)	a = 7.154 b = 7.154 c = 7.302	a = 7.143 b = 7.143 c = 7.301	a = 7.154 b = 7.154 c = 7.312	a =7.177 b = 7.177 c = 7.341	a = 4.095 b = 4.095 c = 5.733	a = 4.106 b = 4.106 c = 20.122	a = 4.077 b = 4.077 c = 5.791
Volume (Å)	323.703	322.685	324,066	327.596	96.172	293.918	96.275
Density (g/cm^3)	6.030	6.001	6,064	6.326	6.127	5.842	6.199
R_p (%)	0.093	0.096	0.098	0.214	0.214	0.214	0.621
R_{wp} (%)	0.133	0.155	0.188	0.271	0.271	0.271	0.708
S	0.98	1.19	1,03	1.02	1.02	1.02	1.28

References

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