Electronic Supplementary Information

$LiBa_{12}(BO_3)_7F_4$ (LBBF) crystals doped with Eu^{3+}, Tb^{3+}, Ce^{3+}: structure and luminescence properties

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Contents

Table S1 Details of data collection and structure refinement for $LiBa_{12}(BO_3)_7F_4$: Eu^{3+} crystal

Crystal data	
Chemical formula	$B_7Ba_{11.72563}F_4LiO_{21}$
M_r	2105
Crystal system, space group	Tetragonal, $P4_2/mbc$
Temperature (K)	293
a, c (Å)	13.5360 (2), 14.9439 (2)
V (Å^3)	2738.07 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	16.67
Crystal size (mm)	0.25 × 0.15 × 0.05
Data collection	
Diffractometer	Esperanto-*CrysAlis PRO*-abstract goniometer imported esperanto images
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.42.49 (Rigaku Oxford Diffraction, 2022) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.182, 1
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	103417, 1987, 1253
R_{int}	0.075
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.694
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.069, 0.65
No. of reflections	1987
No. of parameters	125
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.37, -0.97

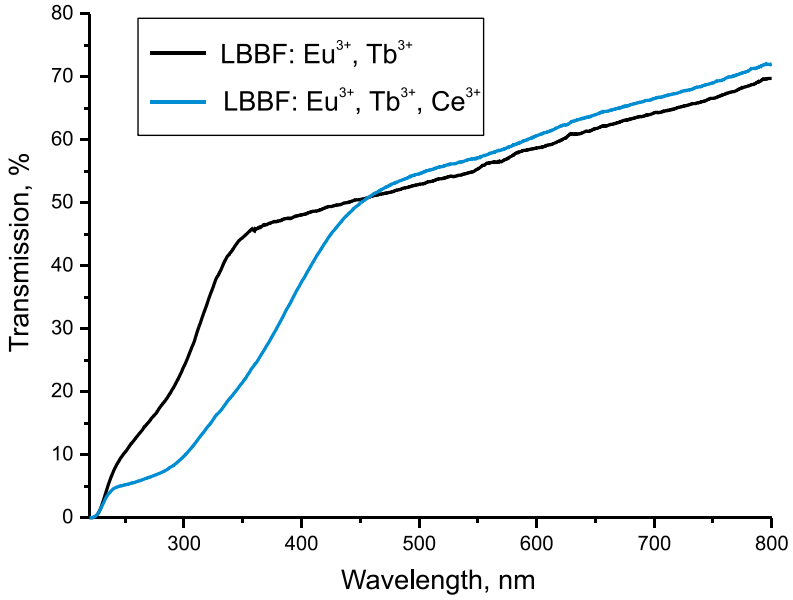


Fig. S1 Transmission spectra of 1.2 mm thick plates made of LBBF: Eu^{3+}, Tb^{3+} and LBBF: Eu^{3+}, Tb^{3+}, Ce^{3+} crystals.

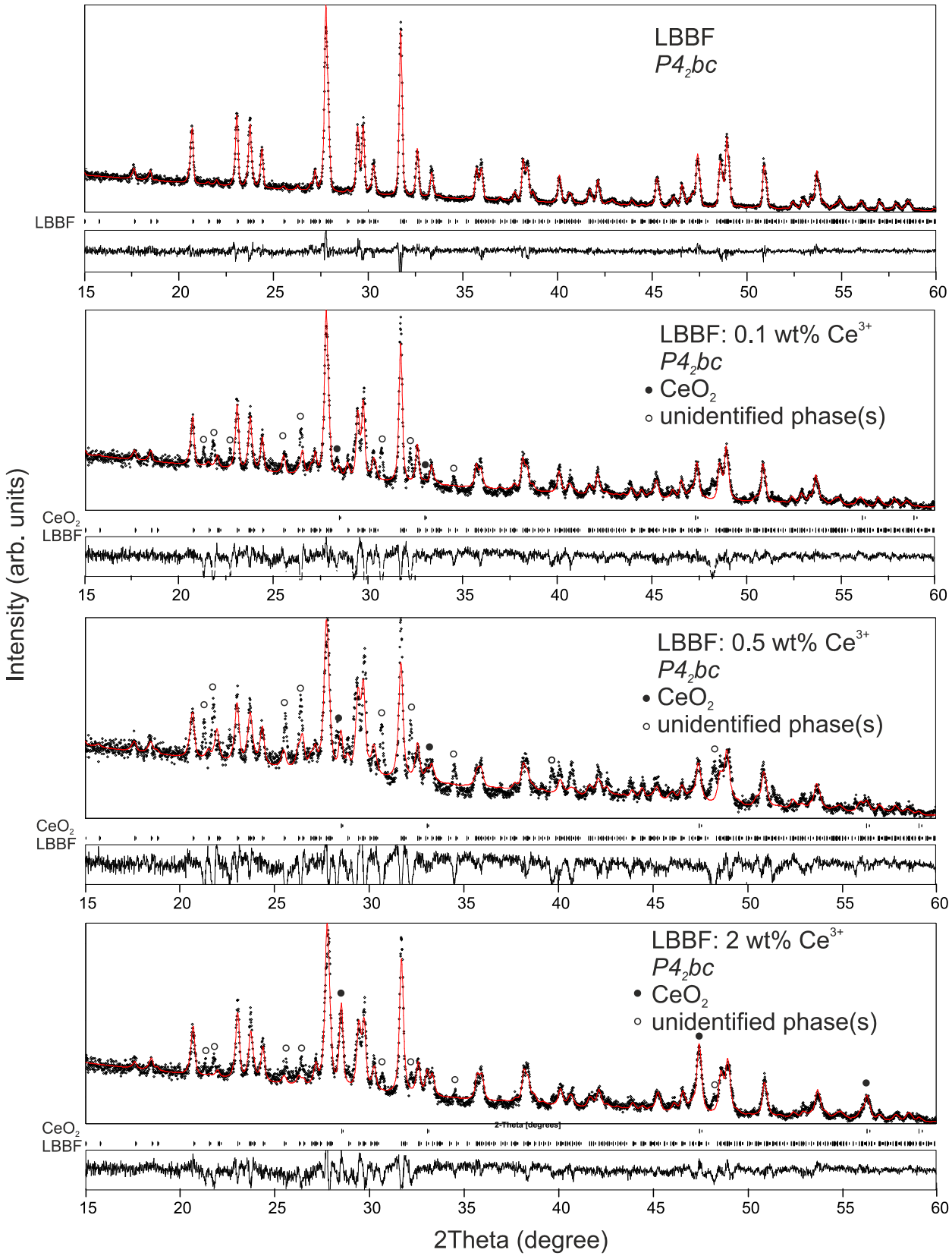


Fig. S2 Rietveld refinement of the X-ray diffraction patterns of solid state synthesized LBBF and LBBF: Ce^{3+} samples.

Table S2 The results of whole-profile fitting of X-ray diffraction patterns of LBBF: Tb^{3+} samples

Phase synthesized by solid-state synthesis	**Space group used for refinement**	**Unit cell parameters, Å**			**V, Å³**	**R_b*, %**
		a	***b***	***c***		
LBBF	$P4_2bc$	13.5464(6)	–	14.9599(8)	2745.2(2)	6.052
LBBF: 0.4 wt% Tb^{3+}	*Pbam*	13.418(1)	13.6523(1)	14.951(1)	2738.9(3)	5.746
LBBF: 0.75 wt% Tb^{3+}	*Pbam*	13.3919(9)	13.688(1)	14.961(1)	2741.5(3)	5.854
LBBF: 1 wt% Tb^{3+}	*Pbam*	13.407(1)	13.669(1)	14.956(1)	2741.1(3)	6.945

R_b* – R-Bragg value for the whole refinement.

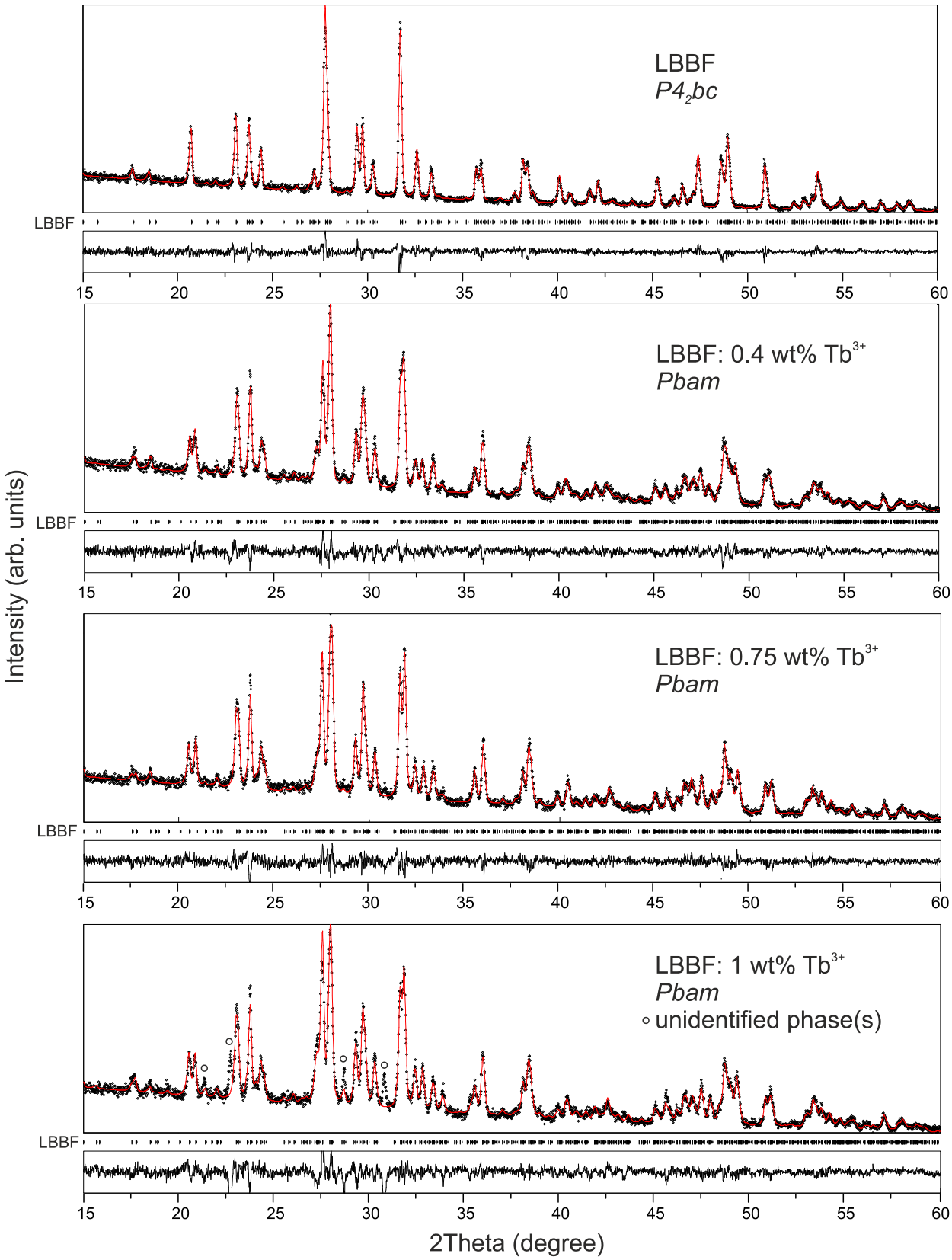
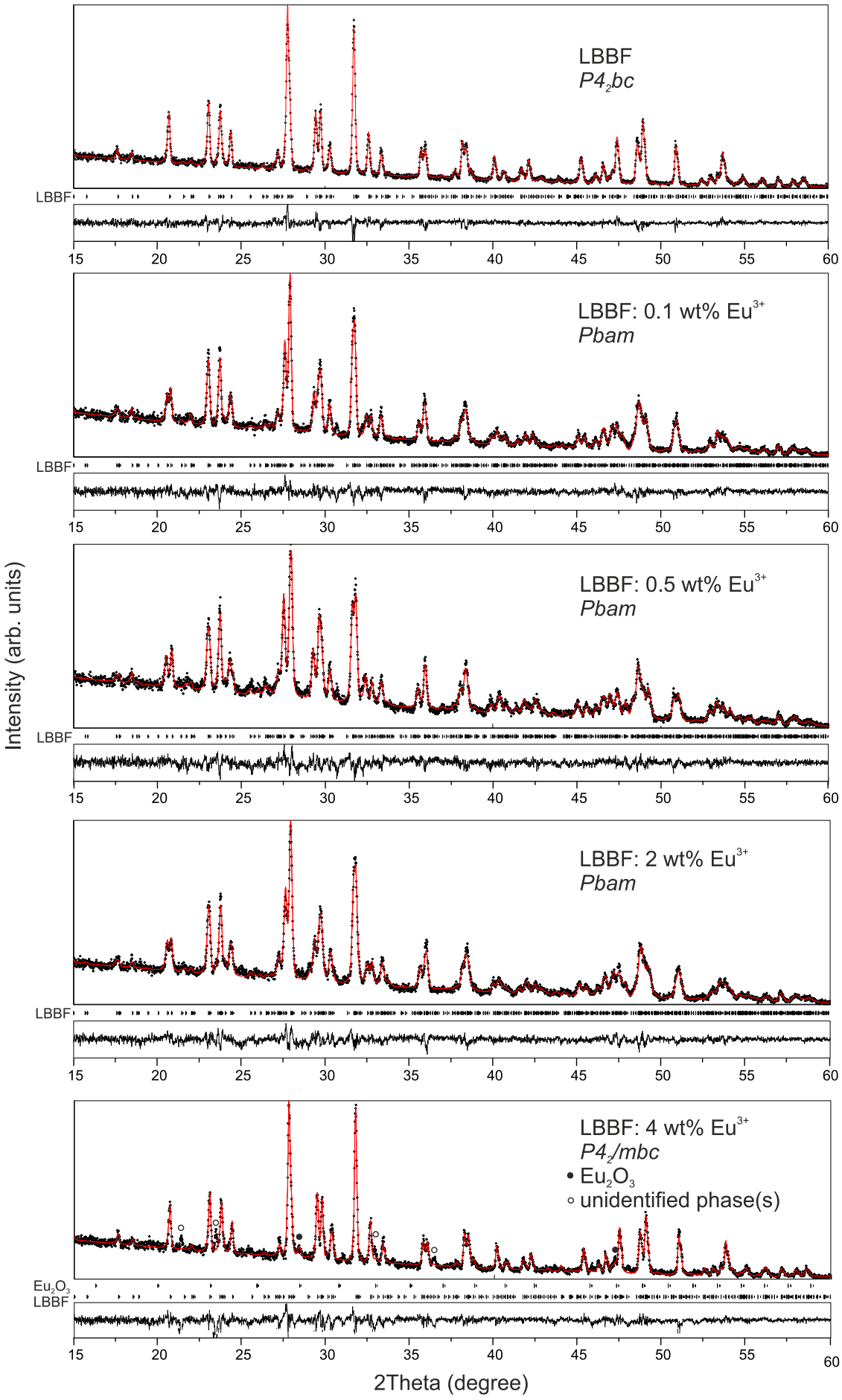


Fig. S3 Rietveld refinement of the X-ray diffraction patterns of solid state synthesized LBBF and LBBF: Tb^{3+} samples.

Table S3 The results of whole-profile fitting of X-ray diffraction patterns of LBBF: Eu^{3+} samples

Phase synthesized by solid-state synthesis	**Space group used for refinement**	**Unit cell parameters, Å**			**V, Å³**	**R_b*, %**
		a	***b***	***c***		
LBBF	$P4_2bc$	13.5464(6)	–	14.9599(8)	2745.2(2)	6.052
LBBF: 0.1 wt% Eu^{3+}	*Pbam*	13.462(1)	13.638(1)	14.974(1)	2749.3(3)	6.002
LBBF: 0.5 wt% Eu^{3+}	*Pbam*	13.421(1)	13.668(1)	14.958(1)	2744.1(3)	5.899
LBBF: 2 wt% Eu^{3+}	*Pbam*	13.450(1)	13.634(1)	14.957(2)	2742.8(3)	6.144
LBBF: 4 wt% Eu^{3+}	$P4_2bc$	13.5393(8)	–	14.950(1)	2740.5(3)	7.567
	Pbam	13.54(1)	13.53(1)	14.951(1)	2740(3)	9.947
LBBF: 5 wt% Eu^{3+}	$P4_2bc$	13.5396(8)	–	14.947(1)	2740.0(3)	7.832
	Pbam	13.540(6)	13.539(7)	14.951(1)	2741(1)	9.111
LBBF: 6 wt% Eu^{3+}	$P4_2/mbc$	13.5398(8)	–	14.948(1)	2740.4(3)	7.831
	Pbam	13.540(7)	13.540(7)	14.951(1)	2741(2)	9.233

R_b* – R-Bragg value for the whole refinement.


LBBF
P4₂bc
LBBF
LBBF: 0.1 wt% Eu3+
Pbam
LBBF
LBBF: 0.5 wt% Eu3+
Pbam
LBBF
LBBF: 2 wt% Eu3+
Pbam
LBBF
LBBF: 4 wt% Eu3+
P4₂/mbc
• Eu2O3
◦ unidentified phase(s)
Eu2O3
LBBF
15 20 25 30 35 40 45 50 55 60
Intensity (arb. units)
2Theta (degree)

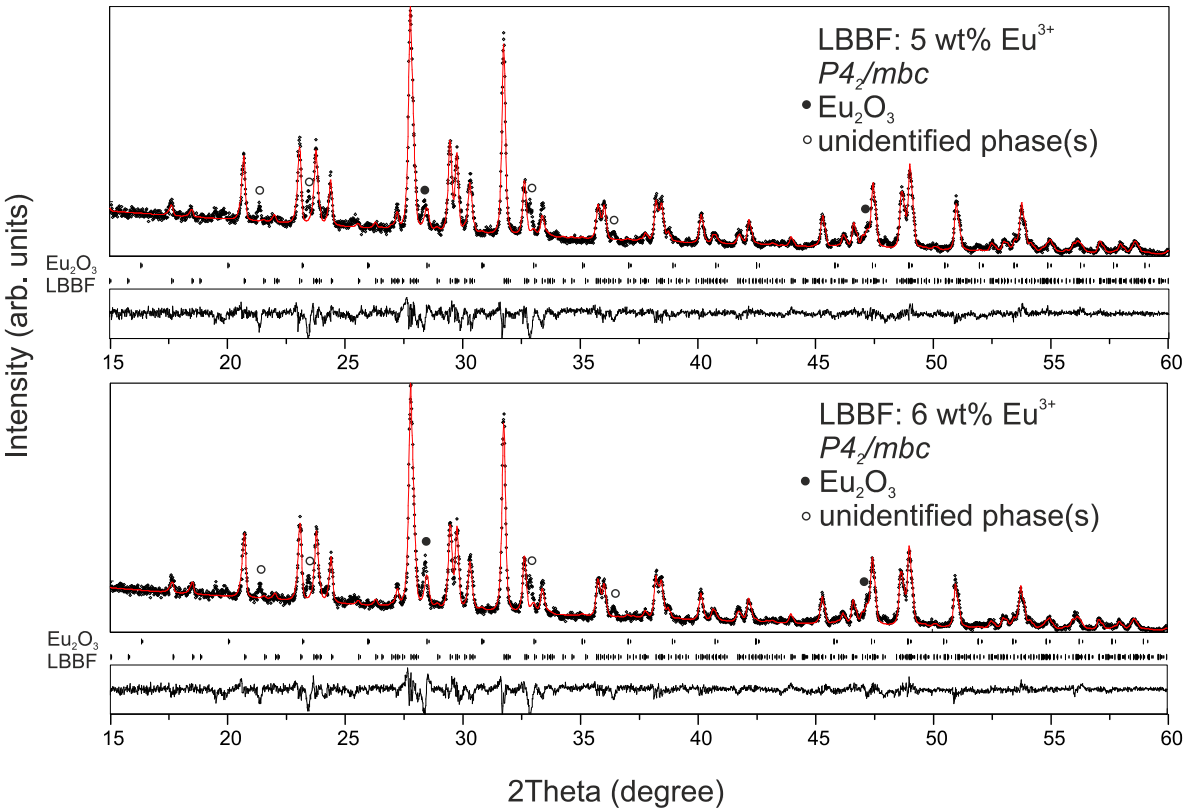


Fig. S4 Rietveld refinement of the X-ray diffraction patterns of solid state synthesized LBBF and LBBF: Eu^{3+} samples.

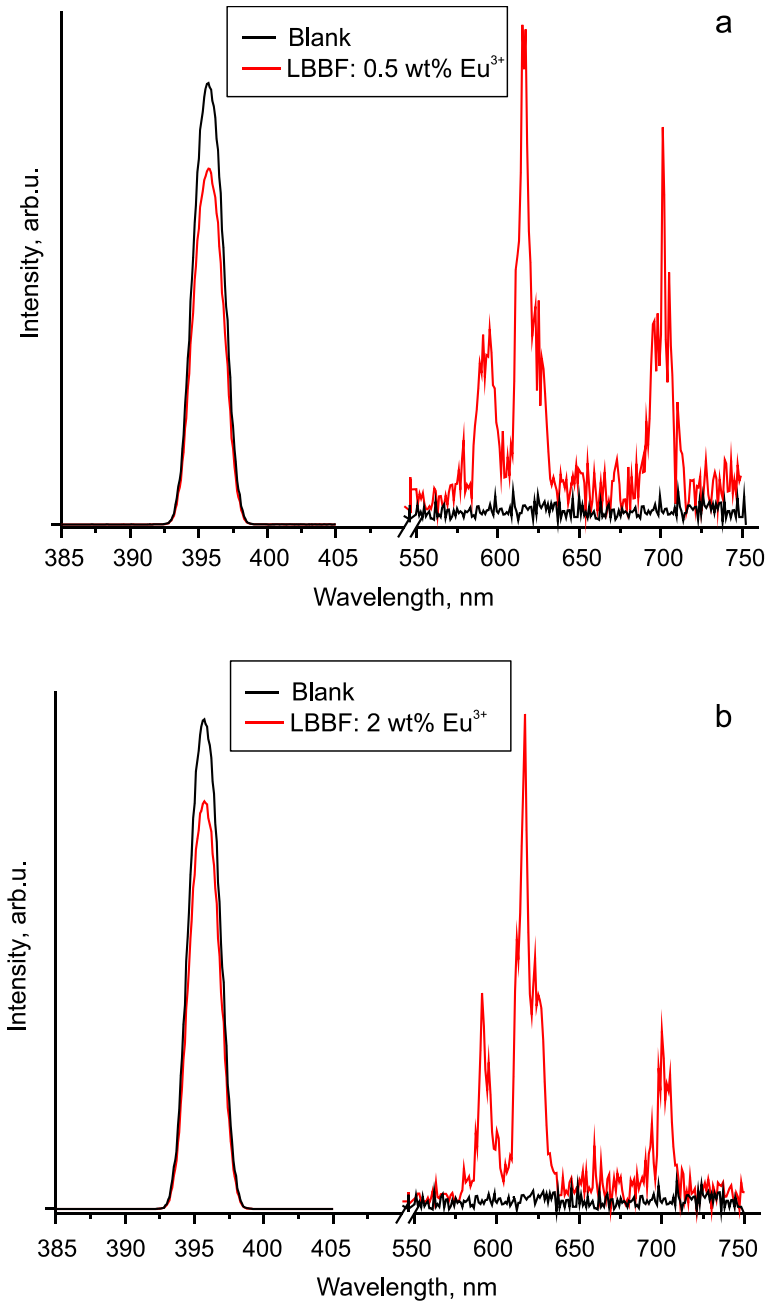


Fig. S5 Excitation light profiles and PL spectra obtained under 395 nm excitation by setting quartz cells with and without the sample: LBBF: 0.5 wt% Eu^{3+} (a), LBBF: 2 wt% Eu^{3+} (b).