

Supporting Information

Effect of annealing on lattice engineering and luminescence in LYSO:Ce scintillators

Ke Xu^{a, b, i, #}, Pan Hu^{a, b, i, #}, Qi Zhang^{c, #}, Qing He^{a, b}, Qingyi Liu^c, Yanan Wang^{a, b, i}, Fazheng Huang^c, Jing Leng^d, Xiaowei Lin^c, Yongcai Shi^{a, b, i}, Kunfeng Chen^{d, *}, Lingyun Li^{c, *}, Juqing Di^{e, *}, Shaowei Feng^{a, b, i}, Qiping Du^{f, g}, Haiyong Ni^h, Dongfeng Xue^{a, b, i, *}

^aShenzhen Institute for Advanced Study, University of Electronic Science and Technology of China, Shenzhen, 518110, PR China

^b University of Electronic Science and Technology of China, Chengdu, 611731, PR China

^c Key Laboratory of Advanced Materials Technologies, International (Hong Kong Macao and Taiwan) Joint Laboratory on Advanced Materials Technologies, College of Materials Science and Engineering, Fuzhou University, Fuzhou, 350108, PR China

^d Institute of Novel Semiconductors, State Key Laboratory of Crystal Materials, Shandong University, Jinan, 250100, PR China

^e Qingyuan Vital Materials Co., Ltd., Qingyuan, 511518, PR China

^f China Rare Earth (Shenzhen) Research Institute Co., Ltd., Shenzhen, 518055, PR China

^g China Rare Earth Group Innovation Technology Co., Ltd., Shenzhen, 518055, PR China

^h Institute of Resources Utilization and Rare Earth Development, Guangdong Academy of Sciences, Guangzhou, 510651, PR China

ⁱSIAS, UESTC-JIREOIMD Joint Institute of Rare Earth Optoelectronic Information Materials and Devices, Shenzhen, 518110, China

* Corresponding authors.

Prof. Dongfeng Xue (dfxue@uestc.edu.cn)

Prof. Kunfeng Chen (kunfeng.chen@sdu.edu.cn)

Prof. Lingyun Li (lilingyun@fzu.edu.cn)

Sr. Eng. Juqing Di (jvqing.di@vitalchem.com)

Table S1 The (Lu/Y/Ce)-O bond electronegativity ($X_{(Lu/Y/Ce)-O}$) and bulk modulus of LYSO:Ce with different Y/Ce content.

x	y	$X_{(Lu/Y/Ce)-O}$	$B(GPa)$
0.0	0.000	0.5253	105.4989
0.0	0.001	0.5253	105.4989
0.0	0.005	0.5253	105.4989
0.0	0.010	0.5252	105.4836
0.0	0.020	0.5251	105.4836
0.1	0.000	0.5244	105.3879
0.1	0.001	0.5244	105.3879
0.1	0.005	0.5244	105.3879
0.1	0.010	0.5244	105.3879
0.1	0.020	0.5243	105.3879
0.2	0.000	0.5236	105.2837
0.2	0.001	0.5236	105.2837
0.2	0.005	0.5236	105.2837
0.2	0.010	0.5235	105.2665
0.2	0.020	0.5235	105.2665
0.3	0.000	0.5228	105.1880
0.3	0.001	0.5228	105.1880
0.3	0.005	0.5227	105.1727
0.3	0.010	0.5227	105.1727
0.3	0.020	0.5226	105.1727
0.5	0.000	0.5211	104.9710
0.5	0.001	0.5211	104.9710
0.5	0.005	0.5210	104.9556
0.5	0.010	0.5210	104.9556
0.5	0.020	0.5209	104.9453

Table S2 The energy resolution (E. R.) and light yield (L.Y.) performance of the unannealed and annealed LYSO:Ce samples.

Samples	E.R. @511 keV (%)	Relative L.Y. @511 keV (a.u.)	E.R. @1.275 MeV (%)	Relative L.Y.@ 1.275 MeV (a.u.)
Unannealed	9.2	24656	14.5	24428
Annealed (1200 °C/10 h)	8.9	37366	8.0	35012

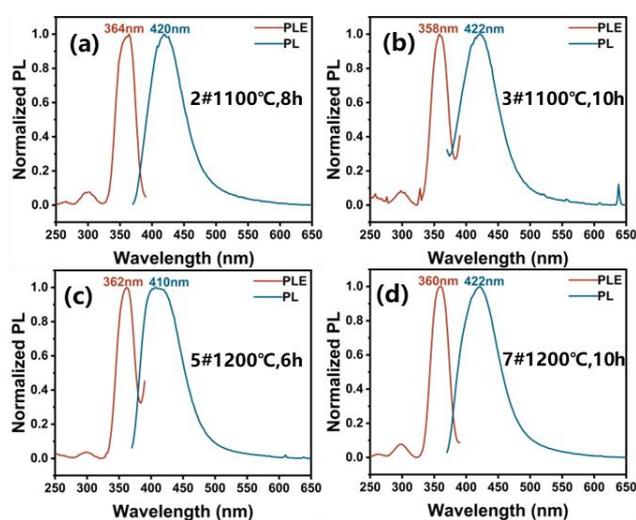


Fig. S1 PLE and PL spectra of LYSO: Ce single crystals which was annealed at (b) 1100 °C for 8 h, (c) 1100 °C for 10 h, (c) 1200 °C for 6 h and (d) 1200 °C for 10 h.

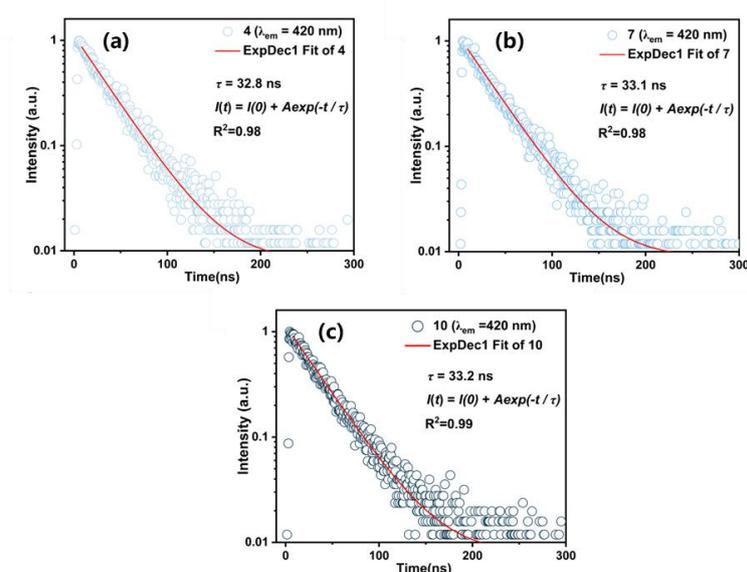


Fig. S2 The fitted decay curve of the luminescence decay curves of LYSO: Ce single crystals which was annealed at (a) 1100 °C for 6 h, (b) 1200 °C for 10 h and (c)

1300 °C for 12 h.

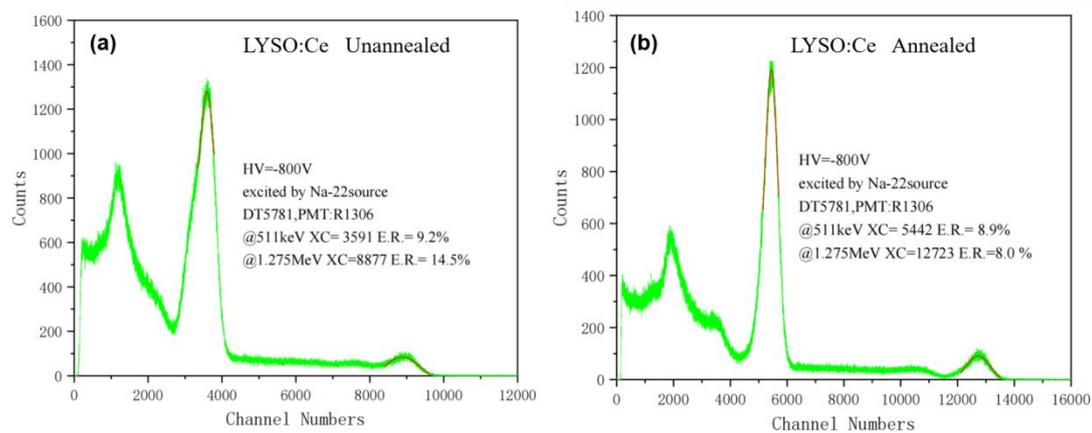


Fig. S3. Typical γ -ray energy spectra of as-grown (a) unannealed and (b) annealed LYSO:Ce samples irradiated by a ^{22}Na source.