

Structure and redshift of Ce³⁺ emission in anisotropically expanded garnet phosphor MgY₂Al₄SiO₁₂:Ce³⁺

Zaifa Pan,^{*,a} Weiqiang Li,^{a,b} Yu Xu,^{a,b} Qingsong Hu^a and Yifan Zheng^{*,b}

^aCollege of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China

^bResearch center of Analysis and measurement, Zhejiang University of Technology, Hangzhou 310014, China

***Corresponding author:**

Zaifa Pan, E-mail: panzaifa@zjut.edu.cn. Phone: 0086-571-88320797

Yifan Zheng, E-mail: zhengyifan@zjut.edu.cn. Phone: 0086-571-88320961

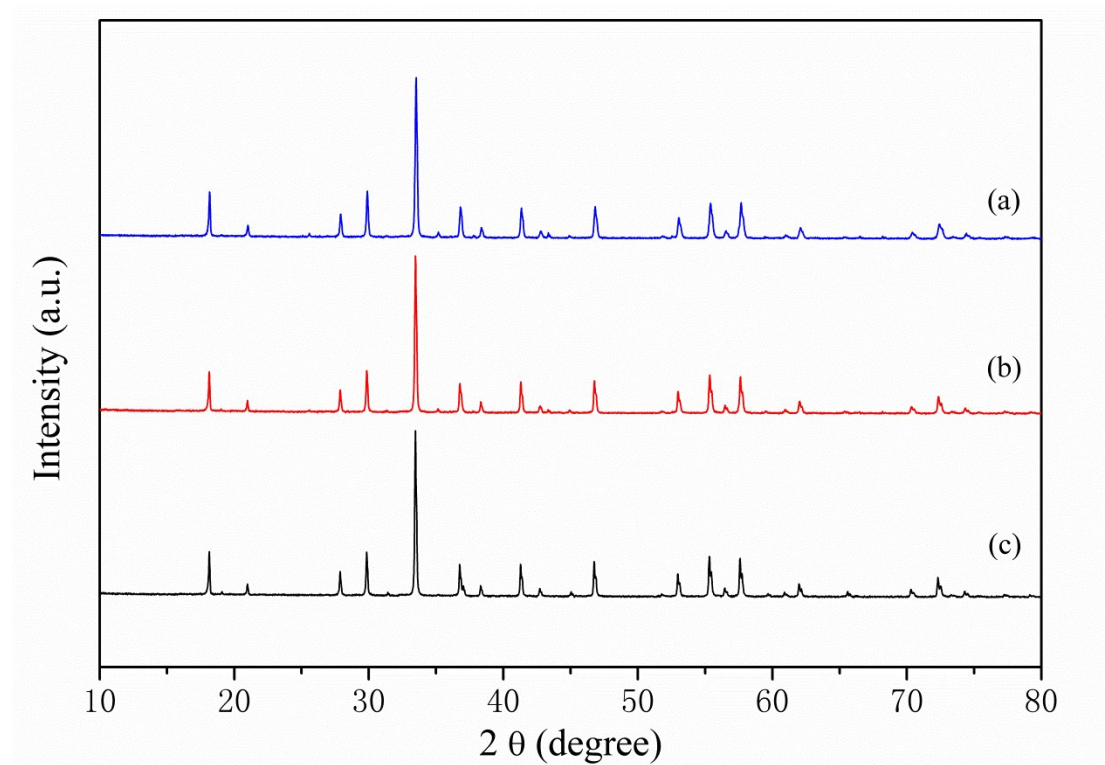


Figure S1 XRD patterns of MYAS:0.06Ce³⁺ synthesized by solid state reaction at 1400 °C (a), 1350 °C (b) and 1300 °C (c).

Table S1 Fractional coordinates, site occupation factors (S.O.F) and thermal vibration parameters of MYAS and YAMS.

atom	site	x	y	x	Occu.	U(Å ²)
MgY₂Al₄SiO₁₂						
Y	24c	0.25	0.125	0	0.667	0.0172
Mg	24c	0.25	0.125	0	0.333	0.0172
Al	16a	0	0	0	1.0	0.0387
Al	24d	0.25	0.375	0	0.667	0.0375
Si	24d	0.25	0.375	0	0.333	0.0375
O	96h	0.0304	0.0538	0.652	1.0	0.0399
Y₃Al₃MgSiO₁₂						
Y	24c	0.25	0.125	0	1.0	0.0125
Mg	16a	0	0	0	0.5	0.00913
Al	16a	0	0	0	0.5	0.00913
Al	24d	0.25	0.375	0	0.667	0.0196
Si	24d	0.25	0.375	0	0.333	0.0196
O	96h	0.250	0.055	0.640	1.0	0.0339
^a Space group: Ia-3d(no.230);; $\alpha=\beta=\gamma=90^\circ$; T=298K; Z=8;Cu K α , $\lambda=1.5418$ nm; lattice parameters: MgY ₂ Al ₄ SiO ₁₂ :a = 11.960 Å, V = 1710.69 Å ³ Rwp=3.91%, Rp=2.51%, $\chi^2=5.810$; Y ₃ Al ₃ MgSiO ₁₂ : a = 12.016 Å, V = 1734.92 Å ³ Rwp=11.74%, Rp=7.27%, $\chi^2=9.787$.						