

Electronic Supplementary Information

Concentration quenching behavior of Stokes and upconversion luminescence for Pr³⁺-doped Y₃Al₅O₁₂

Yuuki Kitagawa,^{†} Hitomi Nakamura,[†] Kenji Shinozaki^{†‡}*

[†]Nanomaterials Research Institute, National Institute of Advanced Industrial Science and Technology
(AIST), Ikeda, Osaka 563-8577, Japan.

[‡]Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan.

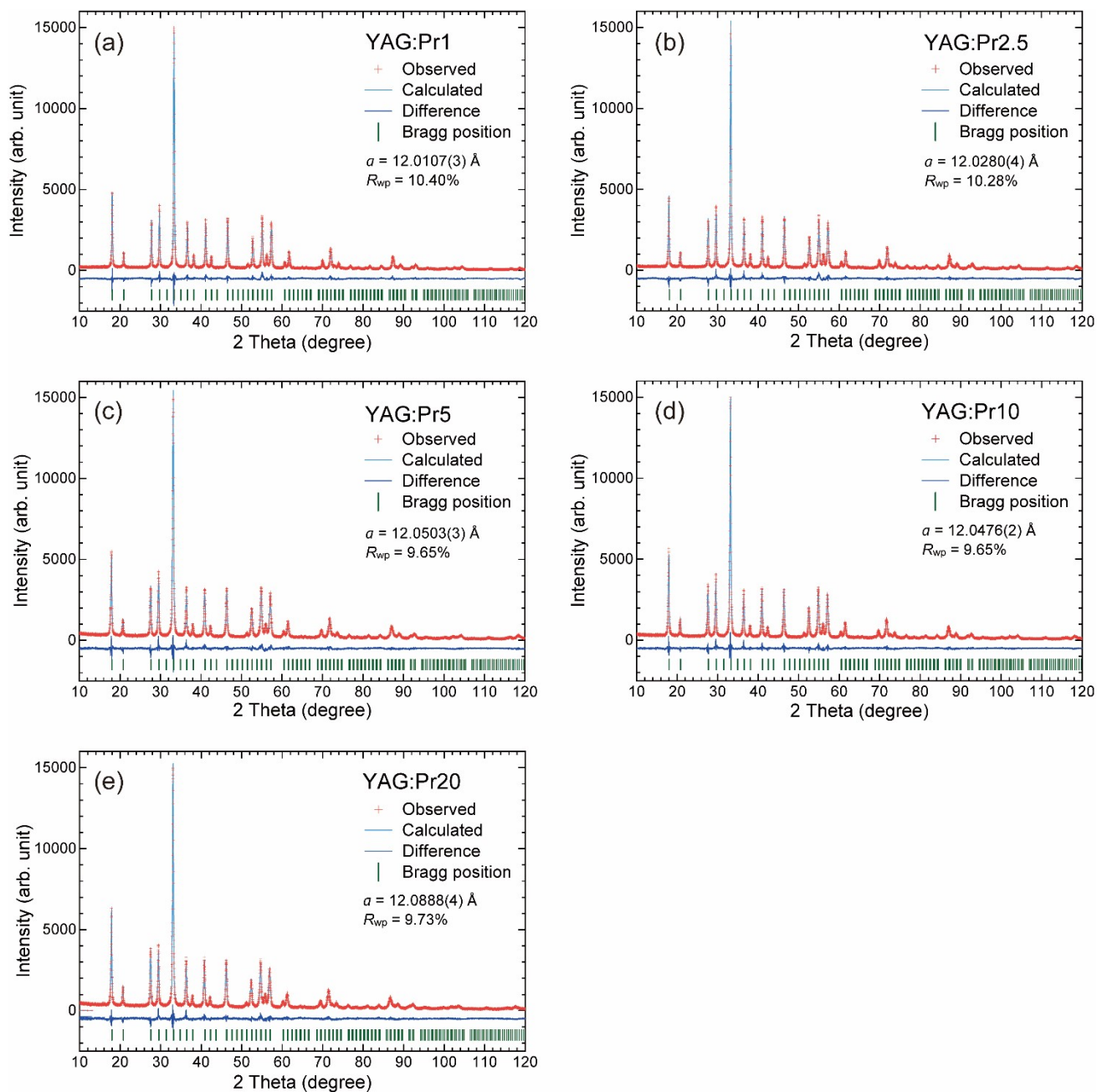


Fig. S1 XRD patterns of the YAG:Pr³⁺ samples with different Pr³⁺ concentrations (1–20%) and the refined plot through the Rietveld method.

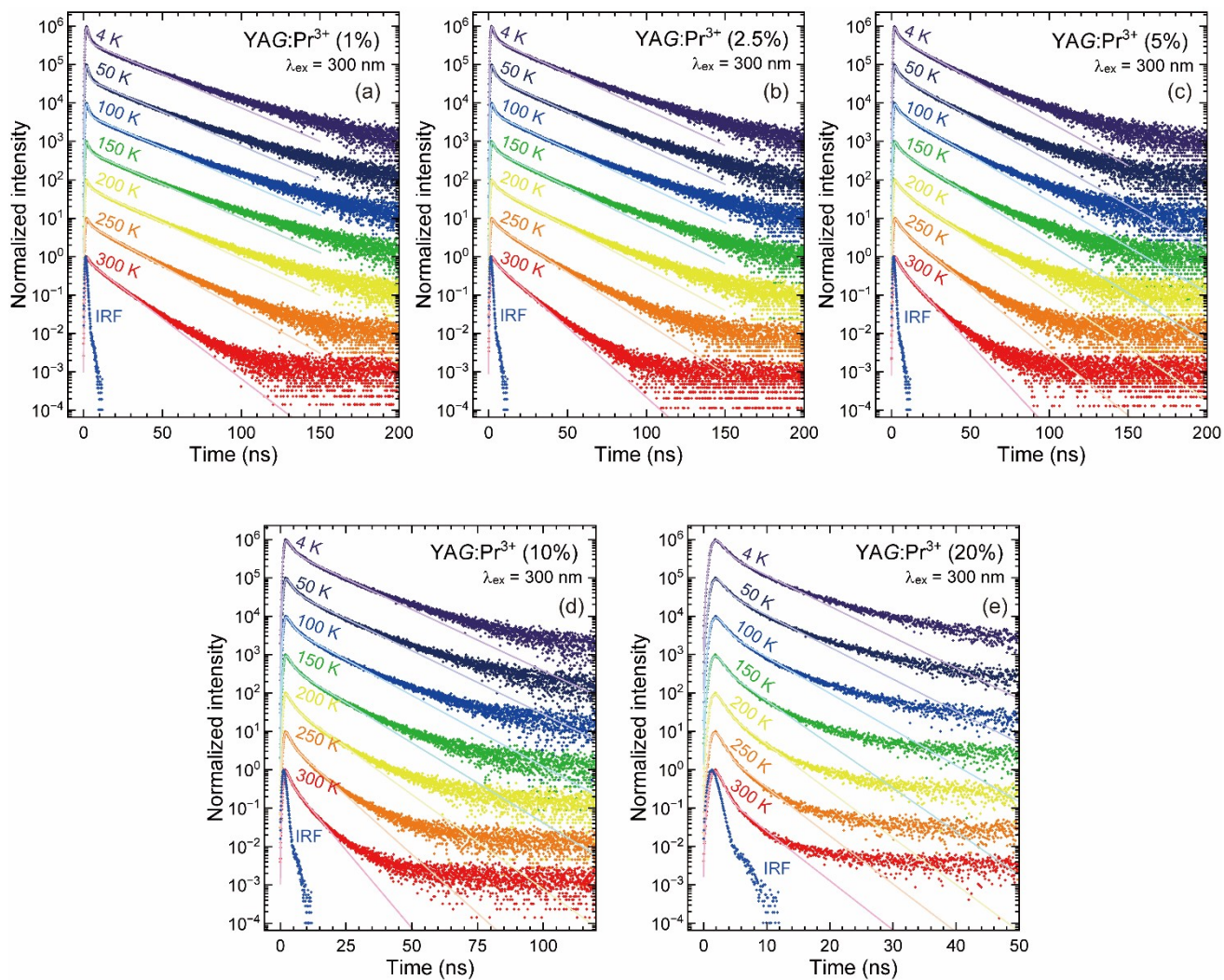


Fig. S2 Temperature dependence of luminescence decay curves of the YAG:Pr³⁺ samples with different Pr³⁺ concentrations (1–20%) and fitting curves using two-component exponential functions. The instrument response functions (IRF) are plotted in blue.

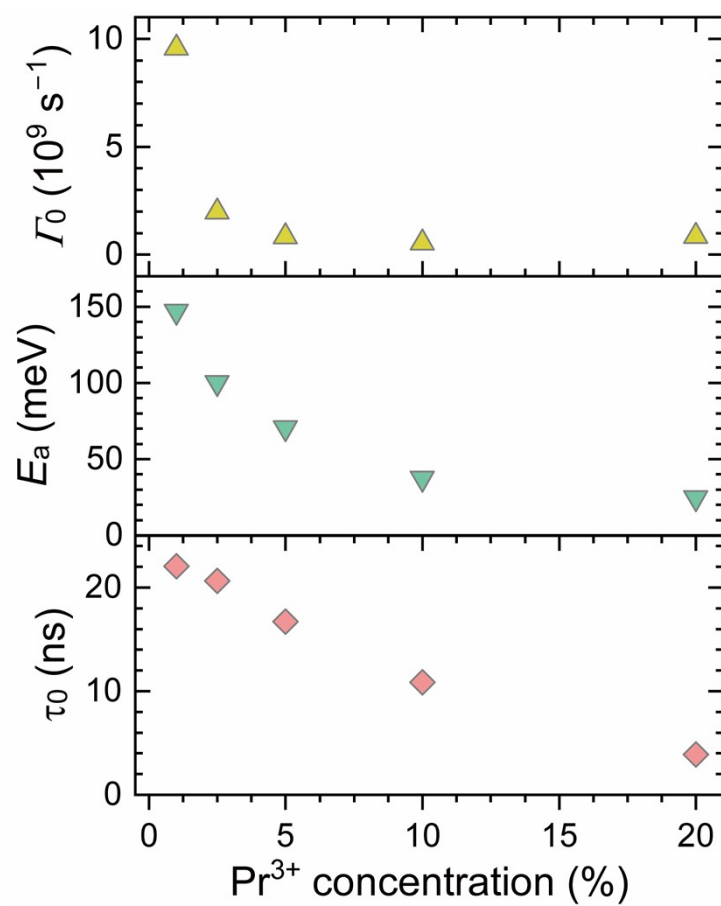


Fig. S3 Pr³⁺ concentration dependence of the attempt rate for the nonradiative transition Γ_0 , the activation energy for thermal quenching E_a , and the fluorescence lifetime τ_0 , which is the reciprocal of the radiative rate Γ_v .

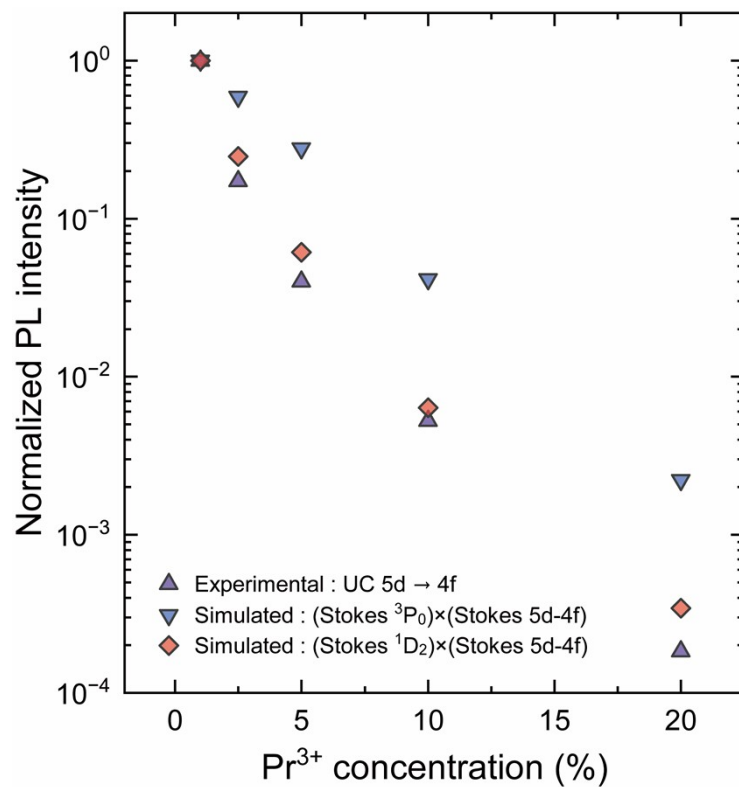


Fig S4 Concentration dependence of Pr³⁺: 5d-4f upconversion luminescence, obtained with the spectroscopic measurements. The simulated plots were the products of the Stokes PL intensities of the 5d-4f and 4f-4f (³P₀ → ³H₄ and ¹D₂ → ³H₄) luminescence, which consider the influence of the cross-relaxation of the intermediate ³P₀ and ¹D₂ states on the upconversion 5d-4f luminescence.

Table S1 Refined structural parameters of the YAG:Pr samples

Sample	YAG:Pr1	YAG:Pr2.5	YAG:Pr5	YAG:Pr10	YAG:Pr20
Chemical formula	Y _{2.97} Pr _{0.03} Al ₅ O ₁₂	Y _{2.925} Pr _{0.075} Al ₅ O ₁₂	Y _{2.85} Pr _{0.15} Al ₅ O ₁₂	Y _{2.7} Pr _{0.3} Al ₅ O ₁₂	Y _{2.4} Pr _{0.6} Al ₅ O ₁₂
Crystal System	Cubic	Cubic	Cubic	Cubic	Cubic
Space group	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$
Lattice constant [Å]	12.0107(3)	12.0280(4)	12.0503(3)	12.0476(2)	12.0888(4)
Z	8	8	8	8	8
R _{wp} [%]	10.40	10.28	9.65	9.65	9.73
R _B [%]	2.76	2.63	2.14	1.93	2.03
S	1.87	1.93	1.99	1.88	2.02

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>g</i>	<i>U</i> _{eq} [Å ²]
YAG:Pr1						
Y, Pr	24 <i>c</i>	0.125	0	0.25	Y: 0.99 Pr: 0.01	0.0358(4)
Al1	16 <i>a</i>	0	0	0	1.0	0.0290(7)
Al2	24 <i>d</i>	0.375	0	0.25	1.0	0.0322(6)
O	96 <i>h</i>	0.4658(1)	0.0481(2)	0.3522(1)	1.0	0.0271(7)
YAG:Pr2.5						
Y, Pr	24 <i>c</i>	0.125	0	0.25	Y: 0.975 Pr: 0.025	0.0319(4)
Al1	16 <i>a</i>	0	0	0	1.0	0.0256(7)
Al2	24 <i>d</i>	0.375	0	0.25	1.0	0.0274(6)
O	96 <i>h</i>	0.4642(1)	0.0472(2)	0.3530(2)	1.0	0.0205(8)
YAG:Pr5						
Y, Pr	24 <i>c</i>	0.125	0	0.25	Y: 0.95 Pr: 0.05	0.0340(4)
Al1	16 <i>a</i>	0	0	0	1.0	0.0279(7)
Al2	24 <i>d</i>	0.375	0	0.25	1.0	0.0294(7)
O	96 <i>h</i>	0.4667(1)	0.0479(2)	0.3528(2)	1.0	0.0241(8)
YAG:Pr10						
Y, Pr	24 <i>c</i>	0.125	0	0.25	Y: 0.9 Pr: 0.1	0.0363(4)
Al1	16 <i>a</i>	0	0	0	1.0	0.0287(7)
Al2	24 <i>d</i>	0.375	0	0.25	1.0	0.0323(6)
O	96 <i>h</i>	0.4669(1)	0.0483(2)	0.3525(2)	1.0	0.0267(8)
YAG:Pr20						
Y, Pr	24 <i>c</i>	0.125	0	0.25	Y: 0.8 Pr: 0.2	0.0380(5)
Al1	16 <i>a</i>	0	0	0	1.0	0.0257(8)
Al2	24 <i>d</i>	0.375	0	0.25	1.0	0.0341(8)
O	96 <i>h</i>	0.4663(1)	0.0483(2)	0.3532(2)	1.0	0.0256(9)