Influence of defect anisotropy on luminescence properties in Pr:YAP crystals: supplement

Lu Zhang (张璐)[1,2], Bowen Jiang (姜博文)[1,3], Mingyan Pan (潘明艳)[1*], Weiguo Ji (纪为国)[1,2], Qiming Fan (范骐鸣)[1,2], Shaoqing Cui (崔少卿)[1,2], Ning Jia (贾宁)[1], Qinglin Sai (赛青林)[1], and Hongji Qi (齐红基)[1,4]**

[1] Advanced Laser and Optoelectronic Functional Materials Department, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China

[2] School of Optoelectronics, University of Chinese Academy of Sciences, Beijing 101400, China

[3] School of Materials and Chemistry, University of Shanghai for Science and Technology, Shanghai 200093, China

[4] Hangzhou Institute of Optics and Fine Mechanics, Hangzhou 311421, China

**Corresponding author: pmy@siom.ac.cn; ** corresponding author: qhj@siom.ac.cn*

The Pr content in the (100), (010), and (001) planes of the Pr:YAP crystal.

The concentration of Pr atom in crystal is determined by ICP-AES method. As can be seen from Table S1, the Pr concentration of the (010) and (001) planes is almost the same, approximately 0.54 at.%. However, the Pr concentration in the (100) plane is 0.45 at.%, significantly lower than that in the other two planes.

Table S1. The elemental content in the (100), (010), and (001) planes of the Pr:YAP crystal.

	(100) plane	(010) plane	(001) plane
Al atom (μg/ml)	228	239	254
Y atom (μg/ml)	751	786	836
Pr atom (μg/ml)	5.4	6.8	7.1

2. The Raman peaks and vibrational modes of the Pr:YAP crystal.

The positions of Raman peaks observed through Raman spectroscopy and their corresponding lattice vibration modes are presented in Table S2.

Table S2. Observed Raman peak positions and their corresponding lattice vibrational modes.

(100) plane (cm^{-1})	(010) plane (cm^{-1})	(001) plane (cm^{-1})	Vibrational modes
148	148	148	A_{1g}
-	-	-	B_{3g}
194	194	194	A_{1g}
214	214	-	B_{2g}
251	254	-	B_{1g}
274	281	274	A_{1g}
305	305	305	B_{2g}
341	341	341	A_{1g}
383	385	385	B_{1g}
409	411	402	B_{2g}

432	432	432	A_{1g}
467	475	-	B_{1g}
522	530	522	A_{1g}
537	-	-	B_{3g}
-	-	-	B_{2g}
550	550	550	A_{1g}

3. Emission spectra (λex=213 nm) of the Pr:YAP crystals

The emission spectra obtained by excitation with a 213 nm (5.82 eV) laser is shown in Fig. S1.

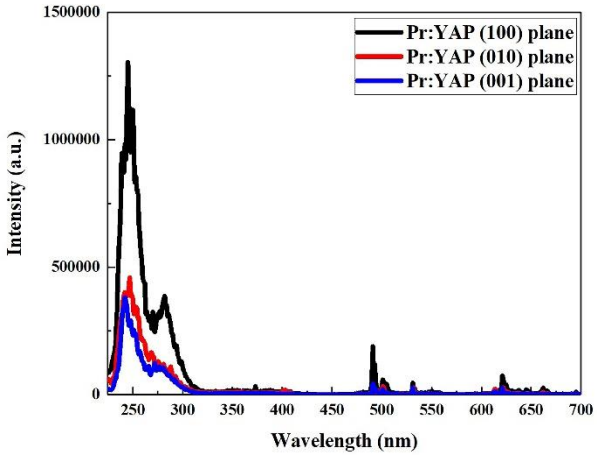

Fig. S1. emission spectra of (100), (010) and (001) crystal plane samples excited by a 213 nm laser.

4. Photoluminescence decay tests of the Pr:YAP crystals

FIG. S2 shows photoluminescence decay tests on (100), (010), and (001) plane samples. The decay times obtained from single-exponential fitting are shown in Table S3. The decay time error is 0.1-0.2 ns. When the excitation wavelength is 213 nm, the nanosecond-scale decay times measured at emission wavelengths of 246 nm and 280 nm are related to the Pr^{3+} $5d_1 \rightarrow 4f$. The excitation wavelength λ_{ex}=213 nm (5.85 eV) surpasses the band gap value of 5.11 eV calculated from the absorption spectra, indicating that the absorption at λ_{ex}=213 nm corresponds to interband absorption in Pr:YAP. The decay times related to Pr^{3+} $5d_1 \rightarrow 4f$ in (100), (010), and (001) planes are approximately 7 ns, which is basically consistent with the photoluminescence decay measured by Zhuravleva[1]. It is found that the decay times for the (100), (010), and (001) planes are almost equal, suggesting the absence of anisotropy in the luminescence mechanism.

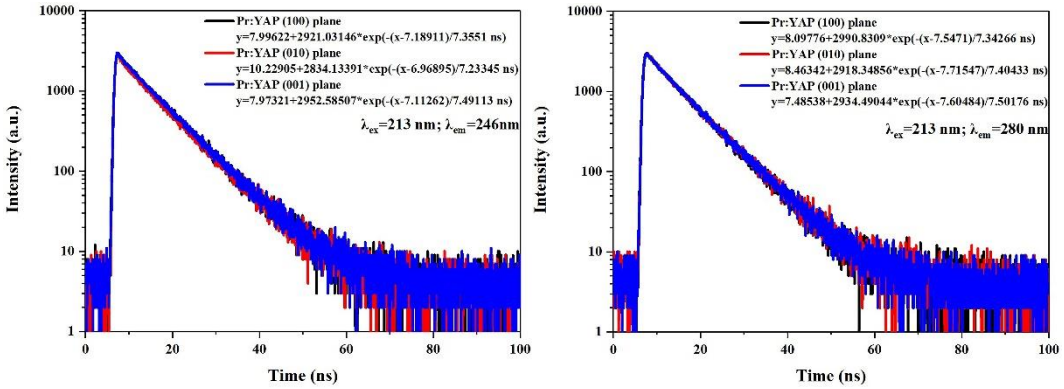

Fig. S2. Photoluminescence decay of (100), (010), and (001) planes at λ_{ex}=213 nm, λ_{em}=246 nm and 280 nm.

Table S3. Photoluminescence decay time of (100), (010), and (001) planes.

Wavelength (nm)	(100) plane (ns)	(010) plane (ns)	(001) plane (ns)
246	7.4	7.2	7.5
280	7.3	7.4	7.5

5. The offset parameters of Al atoms

To elucidate the anisotropic distribution of antisite defects in various crystal planes, relevant calculations are carried out. There are 4 aluminum atoms in the YAP unit cell, and their coordinate positions are shown in Table S4[2]. Through calculations, the average coordinate positions of the Al atoms along the [100], [010], and [001] directions are all 0.25. To quantify the degree of deviation of the Al atoms relative to the (100), (010), and (001) planes, we use the following formula to calculate the offset parameters of the Al atoms[3].

$$\Delta = \frac{p}{n}\sum_{n=1}^{n}\left[\frac{Al_n - < Al >}{< Al >}\right]^2$$

In the formula, Δ represents the offset parameter, Al_n represents the coordinate position of Al atom, <Al> represents the average coordinate position of Al atom, P represents the cell parameters a, b, and c. n is the number of Al atoms in unit cell, which is 4. In Table S4, the offset parameters of Al atoms against (010) and (001) planes are the largest and the smallest, respectively. This demonstrates that Al atoms have a tendency to scatter within the (001) plane, where substitutions of Al atoms by Y atoms are most likely to occur, leading to the formation of defects. Consequently, the (001) plane exhibits the highest probability for the occurrence of antisite defects Y_{Al}.

Table S4. Coordinate positions Al_n, average coordinate positions <Al>, and the offset parameters Δ of Al atom against (100), (010), and (001) planes.

	x/a	y/b	z/c
Al	0.5	0	0
Al	0.5	0	0.5
Al	0	0.5	0
Al	0	0.5	0.5
<Al>	0.25	0.25	0.25
Δ	5.33 (100)	7.37 (010)	5.18 (001)

The cell parameters of YAP are: a=5.329 Å, b=7.370 Å, c=5.179 Å.

Reference

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