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Data Article

Dataset of enhanced UV-C emitting properties of Pr\(^{3+}\)-activated rare earth phosphates driven by structural lattice distortion through a substitutional doping strategy

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Article history:
Received 29 April 2021
Revised 6 May 2021
Accepted 6 May 2021
Available online 17 May 2021

Keywords:
UV-C emission
UV phosphors
Pr\(^{3+}\) doped phosphors
Rare earth phosphate

ABSTRACT

Ongoing global pandemic crisis of coronavirus (COVID-19) and its fast- and wide-spread into entire worlds, critically intimidating our current and future lives, put more emphasis on the development of efficient UV-C emitting phosphors for the germicidal and medical applications due to the intense UV-C emission, which can effectively deactivate such viruses. In this regard, UV-C emitting Pr\(^{3+}\)-activated three presentative rare earth phosphate such as YPO\(_4\), LaPO\(_4\), and La\((x\ \text{mol.}\%\), \(x\ =0-0.21\))-doped YPO\(_4\) have been systematically investigated in terms of crystallographic evolution and their impact on the UV-C emitting properties. Scanning electron microscopy (SEM) images along with X-ray diffraction (XRD) patterns attested the substitutional doping of La into YPO\(_4\) host matrices. Optical properties mainly investigated using the photoluminescence (PL) emission spectroscopy in the spectral range from 220-300 nm corresponding to UV-C energy region clearly demonstrated that the substitutional doping of La into YPO\(_4\):Pr\(^{3+}\) leads to the increase in transition probability of UV-C emission, resulted from the electronic transition of activator corresponding to [Xe]4f\(^5\)5d\(^1\)→[Xe]4f\(^6\). The data presented here are related to the research article entitled “Structural distortion induced enhancement in UV-C emitting properties of Pr\(^{3+}\)-activated La-substituted yttrium phosphates (Y\(_{1-x}\)La\(_x\)PO\(_4\”:Pr\(^{3+}\))”.

DOI of original article: 10.1016/j.jallcom.2021.158707
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https://doi.org/10.1016/j.dib.2021.107145
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Specifications Table

| Subject | Materials Science and Engineering / Inorganic chemistry |
|---------|--------------------------------------------------------|
| Specific subject area | Inorganic Phosphors                                      |
| Type of data | Scheme / Image / Graph                                   |
| How data were acquired | Scanning Electron Microscope, Photoluminescence emission spectroscopy |
| Data format | Raw / Analysed                                           |
| Parameters for data collection | Power type of samples of Pr\textsuperscript{3+}-activated three representative rare earth phosphates YPO\textsubscript{4}, LaPO\textsubscript{4}, and La-doped YPO\textsubscript{4} were mounted on a solid-state sample holder for recording photoluminescence emission spectra |
| Description of data collection | Photoluminescence emission spectra were recorded in the spectral range of 220-230 nm under the variable excitation wavelength from 230-300 nm using a 500W Xenon lamp as a light source |
| Data source location | Institution: Dukungs Women’s University |
| | Country: South Korea |
| | City/Town/Region: Seoul |
| | Latitude and longitude (and GPS coordinates, if possible) for collected samples/data: |
| Data accessibility | https://data.mendeley.com/datasets/rm56r2md7m/3 |
| Related research article | Junsang Cho, “Structural Distortion Induced Enhancement in UV-C Emitting Properties of Pr\textsuperscript{3+}-activated La-substituted Yttrium Phosphates (Y\textsubscript{1-x}LaxPO\textsubscript{4}:Pr\textsuperscript{3+})”, J. Alloys and Compounds, 865 (2021) 158707 |
| | https://doi.org/10.1016/j.jallcom.2021.158707 |

Value of the Data

- The data shows the evolution of optical properties of Pr\textsuperscript{3+} in particular with UV-C emission with varying the La alloying concentration in the YPO\textsubscript{4}:Pr\textsuperscript{3+} inorganic phosphors
- The data provides a fundamental understanding of structure-function correlation in inorganic phosphors: how a lattice distortion induced by La substitution in YPO\textsubscript{4} crystals enhanced the optical emission.
- The data could be used for experiments and further research in the field of inorganic phosphors, providing a fundamental designing principle of inorganic phosphor materials.

1. Data Description

The data presented here are experimental measurements for representative three type of Pr\textsuperscript{3+}-activated YPO\textsubscript{4}, LaPO\textsubscript{4}, and La-doped phosphors with different La concentration, efficiently generating UV-C emission in the spectral range of 230-300 nm due to interconfigurational electronic transition in Pr\textsuperscript{3+} corresponding to [Xe]4f\textsuperscript{4}5d\textsuperscript{1}→[Xe]4f\textsuperscript{2}. A conceptual illustration is depicted in Fig. 1 to demonstrate the formation of single host crystal, solid-solution, and two crystal phase as a function of La substitution concentration (La concentration = 0-21 mol.%). Scanning electron microscope images were collected for Pr\textsuperscript{3+}-activated La(1-8 mol.%)-doped YPO\textsubscript{4} (Fig. 2). The raw data of X-ray diffraction patterns were measured for Pr\textsuperscript{3+}-activated La-doped
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La(PO₄)₃-doped with La(5 mol.%) was prepared as a single host component to Pr-activated YPO₄ samples with 3.5% Pr. The Pr-activated crystalline inorganic phosphors such as YPO₄ (tetragonal), LaPO₄ (monoclinic), and partially La-doped YPO₄ (tetragonal) with an efficient UV-C emission were prepared via the solid-state chemical reaction processes achieved at high temperature (1000°C) for 6 hrs using temperature-controlled electric furnace by following the procedures already reported in the literature precedence. The synthetic procedures for the synthesis of three presentative Pr-activated YPO₄, LaPO₄, and partially La-doped YPO₄ samples are the identical except with using different starting precursors. As an representative example for the synthesis of YPO₄:Pr³⁺, the constituent raw materials of Y₂O₃ (99.9%, High Purity Chemicals), Pr₂O₃ (99.9%, High Purity Chemicals), NH₄H₂PO₄ (99.9%, Kanto Chemicals), were weighed with a stoichiometric ratio. Other Pr³⁺-activated phosphates were also prepared using La₂O₃ (99.9%, High Purity Chemicals) for the synthesis LaPO₄:Pr³⁺ and using the stoichiometrically mixed Y₂O₃ and La₂O₃ for the synthesis La-doped YPO₄:Pr³⁺. Entirely mixed precursors were transfred to the alumina crucible for thermal annealing at atmospheric condition. The photoluminescence (PL) emission spectra were

2. Experimental Design, Materials and Methods

Experimental details, data collection processes have been found in earlier publications [1–4]. The Pr-activated crystalline inorganic phosphors such as YPO₄ (tetragonal), LaPO₄ (monoclinic), and partially La-doped YPO₄ (tetragonal) with an efficient UV-C emission were prepared via the solid-state chemical reaction processes achieved at high temperature (1000°C) for 6 hrs using temperature-controlled electric furnace by following the procedures already reported in the literature precedence [5]. The synthetic procedures for the synthesis of three presentative Pr-activated YPO₄, LaPO₄, and partially La-doped YPO₄ samples are the identical except with using different starting precursors. As an representative example for the synthesis of YPO₄:Pr³⁺, the constituent raw materials of Y₂O₃ (99.9%, High Purity Chemicals), Pr₂O₃ (99.9%, High Purity Chemicals), NH₄H₂PO₄ (99.9%, Kanto Chemicals), were weighed with a stoichiometric ratio. Other Pr³⁺-activated phosphates were also prepared using La₂O₃ (99.9%, High Purity Chemicals) for the synthesis LaPO₄:Pr³⁺ and using the stoichiometrically mixed Y₂O₃ and La₂O₃ for the synthesis La-doped YPO₄:Pr³⁺. Entirely mixed precursors were transfred to the alumina crucible for thermal annealing at atmospheric condition. The photoluminescence (PL) emission spectra were

| La 0 mol.% | La 1-5 mol.% | < La 5 mol.% |
|------------|--------------|--------------|
| Single Component YPO₄:Pr³⁺ | Solid Solution Y₁ₓLaₓPO₄:Pr³⁺ | Heterogeneous formation YPO₄:Pr³⁺ & LaPO₄:Pr³⁺ |

Fig. 1. Schematic illustration of the formation for UV-C emitting Pr³⁺-activated rare earth phosphates as a function of La substitution (x mol.%), indicating that the increase of an amount of La substitution in YPO₄:Pr³⁺ (single host component) leads to the formation solid solution (Y₁ₓLaₓPO₄:Pr³⁺) at the relative low La concentration (La 1-5 mol.%) and further increase results in heterogeneous formation of the LaPO₄:Pr³⁺ at the higher concentration of La (> 5 mol.%).

Fig. 2. Scanning electron microscope (SEM) images for Y₁ₓLaₓPO₄:Pr³⁺ as a function of La concentration (x mol.%) from La 1-8 mol.% (x = 0.01-0.08).

YPO₄ with different La concentration (1-25 mol.%) as shown in Fig. 3. As a representative example, the photoluminescence emission (PL) spectra were recorded for Pr³⁺-activated La(5 mol.%) doped YPO₄ under the variable excitation wavelength from 220–230 nm (220, 223, 225, 228, 230 nm) along with the energy diagram for the excitation and emission processes (Fig. 4A,B). The PL emission spectra were recorded under excitation wavelength of 225 nm for Pr³⁺-activated La(x mol.%) doped YPO₄ as a function of varying La concentration (Fig. 5). Scanning electron microscope images for the samples of Pr³⁺-activated YPO₄, LaPO₄, and La(5 mol.%) doped YPO₄ were taken while measuring the cathodoluminescence emission spectra for the sample (Fig. 6).
Fig. 3. X-ray diffraction (XRD) patterns acquired for $\text{Y}_{1-x}\text{La}_x\text{PO}_4:\text{Pr}^{3+}$ upon varying the La concentration from 1-21 mol.%. The bottom red tick mark corresponds to tetragonal YPO$_4$ (PDF# 01-084-0335) whereas blue tick marks represent the monoclinic LaPO$_4$ (PDF# 01-084-0600).

Fig. 4. Photoluminescence emission (PL) spectra for Pr$^{3+}$-activated La (5 mol.%)-doped YPO$_4$:Pr$^{3+}$ (Pr$^{3+}$ 3 mol.%) under the different excitation wavelength of 220, 223, 225, 228, and 230 nm. The excitation energy (or wavelength) determines the fate of photoluminescence emission processes and emission intensity.

recorded by PSI Instruments equipped with DarsaPro 5000 using a 500W Xenon lamp as an excitation source. Scanning electron microscope images were taken using Tescan Mira 3 LMU FEG, which was operated at an accelerating voltage of 10 kV. X-ray diffraction patterns were collected using the X-ray diffractometer of Rigaku D/Max-2200V in a 2 theta range from 20-60° with a step size of 0.02; the X-ray source is based on Cu Kα radiation with corresponding wavelength of 0.15405 nm.
Fig. 5. Photoluminescence emission (PL) spectra acquired for Pr\textsuperscript{3+}-activated La (x mol.\%)-doped YPO\textsubscript{4}:Pr\textsuperscript{3+} (Pr\textsuperscript{3+} 3 mol.\%) as a function of La concentration varied from 0-25 mol.\% (x = 0-0.25) under the excitation wavelength of 225 nm shown in panel A. The PL intensity displayed in panel B represents the integrated PL area intensity under each PL spectrum shown in panel A ranging from 230-300 nm.

Fig. 6. Scanning electron microscope (SEM) images obtained for YPO\textsubscript{4}:Pr\textsuperscript{3+}, LaPO\textsubscript{4}:Pr\textsuperscript{3+}, La(5 mol.\%)-doped YPO\textsubscript{4}:Pr\textsuperscript{3+} while recording the cathodeluminescence emission spectra at the accelerating voltage of 10 kV with magnification of 2500 X.

**Ethics Statement**

The study does not contain any research involving human participants and/or animals performed by any of the author.

**CRediT Author Statement**

**Junsang Cho:** Conceptualization, Methodology, Experiment, Data analysis, Writing - Original Draft Preparation, Investigation, Supervision, Software, Writing - Reviewing and Editing.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

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