Effects of anisotropy on structural and optical characteristics of LYSO:Ce crystal

Dongzhou Ding*,1,2, Jianhua Yang1,2, Guohao Ren1,2, Martin Nikl3, Sheng Wang, Yuntao Wu1,2, and Zhiyong Mao1

1 Shanghai Institute of Ceramics, Chinese Academy of Sciences, No. 1295 Dingxi Road, Shanghai 200050, P. R. China
2 Research and Development Center of Shanghai Institute of Ceramics, No. 588 Heshuo Road, Shanghai 201899, P. R. China
3 Institute of Physics, Academy of Sciences of The Czech Republic, 162 53 Prague, Czech Republic

Received 18 November 2013, revised 2 March 2014, accepted 4 March 2014
Published online 7 April 2014

Keywords: anisotropic properties, LYSO:Ce, optical properties, scintillation crystals, structural properties

* Corresponding author: e-mail dongzhou_ding@mail.sic.ac.cn, Phone: +86 21 69906301, Fax: +86 21 59927184

In this paper, Cerium-doped lutetium yttrium oxyorthosilicate crystal (Lu,Y)2SiO5:Ce (LYSO:Ce) samples were used to thoroughly investigate the structural and optical anisotropy of the crystal. Results presented demonstrate that there is insignificant anisotropy in most of the properties of LYSO:Ce crystal – structural integrity, refractive index, transmittance, excitation and emission spectra, and photoluminescence decay time, which is a comparative advantage for various applications including preparation of optical ceramics. Besides, anisotropy phenomena in fine-structure of LYSO:Ce, afterglow, thermoluminescence and light output of samples with small size were observed. A mechanism of anisotropy in defect distribution is discussed.

1 Introduction Non-cubic crystal structures usually show anisotropic character not only in the crystal growth [1, 2] but also in various properties [3, 4] due to the directional arrangement of the lattice constituents. For example, tetragonal scheelite lead tungstate (PbWO4) crystal shows strong anisotropy in scintillation properties and refractive index, which results in strong directional dependence of theoretical limit of transmittance [5–8]. The research on the anisotropy in optical performance and scintillation properties of single crystals is helpful for both the growth process and its applications.

Cerium-doped lutetium oxyorthosilicate crystal (Lu2SiO5:Ce, namely LSO:Ce) became of interest in the early 1990s, owing to its excellent scintillation properties [9, 10]. In the past decade, Cerium-doped lutetium yttrium oxyorthosilicate crystal ((Lu,Y)2SiO5:Ce, namely LYSO:Ce) has attracted extensive attention due to the advantages of lower melting point, cheaper starting material, a reduced amount of defects, etc. [11–15], and has been extensively studied as a promising scintillator in the application fields including nuclear medicine [16–19] and high-energy physics [20–23]. LYSO:Ce has monoclinic structure; its space group is C2/c. The angle of β is about 122.2°. There is a large difference in cell parameter axes a, b, and c as well. The structural symmetry of LYSO:Ce is low. It was once reported that LSO:Ce has obvious anisotropy in its thermal expansion [24–26] and thermal conductivity [25]. However, there is still no systematic study of the influence of structural anisotropy on the other material characteristics in LYSO crystal.

In the early stages of this research, we observed that the light output is anisotropic for the oriented LYSO crystal sample (see Section 3.6 of this paper). However, our experimental results also proved that the light output is isotropic for an unoriented cubic LYSO crystal sample with the dimension of 20 × 20 × 20 mm³. We were interested to...
find out the contributing factors to the origin of such a phenomenon.

In this paper, the anisotropy of microstructure, structural integrity, refractive index, transmittance, photoluminescence, afterglow, and thermoluminescence characteristics as well as light output in LYSO crystal were investigated systematically.

2 Experimental

2.1 Sample preparation

LYSO:Ce crystal was spontaneously grown from the melt with composition of (Lu0.9Y0.1)2SiO5:Ce by using Czochralski method in atmosphere of nitrogen. For further details see Ref. [14]. The grown LYSO crystal is colorless and clear, without any visible inclusions. The actual Lu, Y contents in the grown crystals were analyzed by X-ray Fluorescence (XRF) measurements (Philips PW2404). The cerium concentration was determined by inductively coupled plasma optical emission spectroscopy (ICP-OES, Varian Vista Pro, USA).

According to the relevant data from the Inorganic Crystal Structure Database ICSD-279584 [27], crystallographic faces (200), (020), and (002) were determined using an Aolong YX-2 X-ray diffractometer. The oriented crystal was cut from the LYSO:Ce ingot.

For the convenience of anisotropy investigation, the outer part of the oriented LYSO crystal was sliced into two sets of samples with dimensions of 15 x 10 x 2 mm³ and 5 x 5 x 0.5 mm³. The larger surface (15 x 10 mm² or 5 x 5 mm²) is one of the three principal crystallographic faces (200), (020), or (002). As listed in Table 1, the samples with dimension of 15 x 10 x 2 mm³ (Fig. 2a) were used for the measurements of surface morphologies, Raman spectra, X-ray rocking curves, transmittance spectra, afterglow curves, fluorescence decay curves, photoluminescence excitation and emission spectra. The samples with dimension of 5 x 5 x 0.5 mm³ were used for thermoluminescence measurements.

The inner part of the oriented LYSO crystal was cut into two samples. The one with more right angles (Fig. 5b) (dimensions 19 x 10 x 6 mm³) was used for refractive index measurements. The other one was used for transmittance and light output measurements (Fig. 2a) (dimensions 16 x 16 x 16 mm³). It was cut into the shape with crystal surfaces as (200), (020), and (002). The areas of these faces were the same as 297 mm²; the thicknesses in directions vertical to these three faces were the same as 16 mm (Fig. 2a).

In short, all the samples used in this study were cut from the same portion of the same LYSO ingot. They were mechanically polished to a high optical grade (see Figs. 2 and 7) using the same procedure. The surface morphologies were determined by atomic force microscopy (AFM, Nanocute SII, Seiko, Japan) at dynamic force microscopy (DFM, tapping mode) with scan speed 1 Hz (Fig. 2b).

2.2 Structure measurements

Single-crystal X-ray diffraction (SCD) structure analysis data were collected using a CAD4 Diffractis-586 single-crystal X-ray diffractometer (Enraf-Nonius). The unpolarized Raman spectra were recorded with Renishaw inVia Raman microscope. The X-ray rocking curves of the samples were recorded with a Bruker D8 Discover X-ray diffractometer at 40 KV and 40 mA.

2.3 Refractive index and transmittance measurements

The refractive indices were recorded with KALNEW KPR-2000 precision refractometer. To reduce error in measuring refractive index, LYSO crystal samples were coupled to V-prism with contact liquid, whose refractive index is 1.77, which is close to the refractive index of LYSO. The optical transmittance spectra were measured by using a Hitachi U-3900H spectrophotometer (scan speed: 300 nm min⁻¹; slit width: 4 nm; sampling interval: 1 nm).

2.4 Luminescence and scintillation property measurements

The fluorescence decay curves, the photoluminescence excitation and emission spectra were recorded with an Edinburgh FLS-920 spectrophotometer with a nano-second hydrogen-filled flashlamp. The LYSO crystal sample (16 x 16 x 16 mm³) for light output (L.O.) measurements was wrapped with enhanced specular reflector (ESR) made by 3M company. Different oriented surfaces of the same sample were selected respectively as the coupling surface, and coupled to a R878 photomultiplier tube (Hamamatsu) with air. 662 KeV gamma ray from a ¹³⁷Cs source was used to excite the sample and then pulse-height (energy) spectra were recorded by an ORTEC digiBASE multichannel spectrometer.

2.5 Afterglow and thermoluminescence measurements

Afterglow was measured under X-ray pulse excitation and the decay profiles were recorded at the oscilloscope (Tektronix DPO 5104) using a photomultiplier tube (PMT, R669) photodetector. Thermoluminescence (TL) measurements after RT X-ray irradiation were performed from room temperature (RT) to 500 °C with a linear heating rate of 1 °C s⁻¹ by using a ROSB TL/OSL 3DS (Guangpeng) wavelength resolved TL spectrometer.
Experimental conditions and geometry were kept carefully the same when mutual intensities of the samples were to be compared quantitatively. All but TL measurements were carried out at RT.

3 Results and discussion

The XRF result shows the actual composition of the crystal grown from the melt with composition of \((Lu_{0.9}Y_{0.1})_2SiO_5:Ce\) is \((Lu_{0.913}Y_{0.087})_2SiO_5:Ce\). The difference between melt and crystal compositions results from the dopant segregation due to the larger radius of \(Y^{3+}\) than that of \(Lu^{3+}\). The ICP-OES results show the nominal and the actual Cerium concentration within the crystal are 0.4 and 0.1 at%, respectively.

Figure 1 shows that the measured diffraction angle \(\theta\) values of LYSO crystal for planes (200) and (020) are 7.25° and 13.51°, respectively, which are very close to the reference values of LSO with difference less than 0.1°, indicating a good orientation accuracy. However, the orientation accuracy of crystal plane (002) is poor as compared with that of crystal planes (200) and (020), and the difference between measured and reference values is 1.06°. This can be ascribed to the fact that (002) plane has a weaker diffraction intensity \((I = 5\%)\), making it more difficult to orientate the crystal during production.

The oriented LYSO crystal with three principal crystallographic faces has a rhombus external appearance (Fig. 2a). To investigate the 3D surface topography, atomic force microscopy images were taken by scanning (200), (020), and (002) crystal surfaces, each in an area of \(6 \times 6\) µm². As shown in the surface profiles in Fig. 2b, root-mean-square (RMS) surface roughness values of these oriented planes are 1–5 nm, almost the same as those of mechanically polished LSO (2–4 nm) [28]. The small roughness indicates that the planes were very well polished. Besides, it is worth mentioning that in spite of the same mechanical polishing procedure, the surface roughness value of (200) is smaller than that of (020) and (002). The possible reason for this lies in the fact that there happened to be no deeper scratch in the randomly selected measured region of (200) as those shown in (020) and (002).

3.1 Anisotropy in fine structure

The “Anisotropy in Fine-structure” was investigated by “unpolarized Raman spectra.” As shown in Fig. 3, the Raman spectra of LYSO crystal for (200), (020), and (002) plane can be divided into three different parts [29, 30]: the 0–300 cm⁻¹ low wave-number region (I) (corresponding to the motion of the cations with respect to the whole structure), the 300–800 cm⁻¹ region (II) (corresponding to the vibrations of Re–O), and the 800–1000 cm⁻¹ region (III) (corresponding to
to the vibrations Si–O atoms). Differences in peak intensities, widths and positions for the Raman spectra of three LYSO crystal planes (200), (020), and (002) are observed, implying the significant anisotropy of molecule’s vibration, rotation and symmetry property for LYSO fine-structure.

The crystal structure was analyzed by Single-crystal X-ray diffraction. By using the SCD data, the LYSO cell parameters were calculated as $a = 14.263(3)$ Å, $b = 6.6346(12)$ Å, $c = 10.2421(18)$ Å, $\beta = 122.202(2)^\circ$ and $\alpha = \gamma = 90^\circ$. The space group was determined to be $C2/c$, which is the same as that of LSO [27], indicating that the substitution by yttrium does not change the structural symmetry of LSO.

We define areal ion density as the number of ions “involved” (actually not exactly involved, but treating all those ions in unit cell as “involved” in the studied plane) in unit area, i.e., areal ion density equals the number of ions divided by the area of the plane. With this definition, we can give a qualitative comparison of ion density in different planes. By using the cell parameters shown above, the areas of (200), (020), and (002) – the three principal planes – in the unit cell were respectively calculated to be 68.068, 123.71, and 94.663 Å$^2$. The number of ions in the unit cell being the same (64, $Z = 8$), the relative areal ion density ratio of these three planes equals $64/68.068 : 64/123.71 : 64/94.663$. The ratio was normalized to the highest one – the areal ion density of (200). In this way, the calculated ratio is 100%:55%:72%. It is clear that (200) and (020) have, respectively, the highest and the lowest areal ion density among these three planes.

### 3.2 Anisotropy in structural integrity

The concept “structural integrity” was used in this work to characterize the perfection of the single crystal structure of LYSO:Ce. A crystal sample with high structural integrity indicates it has a rather perfect structure with less lattice distortion. The anisotropy in integrity was investigated by “Maps of rocking curve.” We measured rocking curves every other 1 mm in these faces.

As shown in the maps of rocking curve widths (full width at half maximum, shortened as FWHM) for these three faces (Fig. 4), the Bragg peaks’ FWHM distribution varies slowly, indicating a good homogeneity of structural integrity and the absence of abrupt macroscopic defective areas. From small Bragg peak widths (around 20 arcsec), we conclude that the oriented LYSO samples depicted in Fig. 4 are of very high structural integrity. Since the values of FWHM are almost the same for all the three faces, it is reasonable to say the anisotropy in integrity is insignificant.

### 3.3 Anisotropy in refractive index

Refractive index is an important parameter for scintillation crystals. It affects transmission characteristics of light in crystals and light collection efficiency at the photodetector [31]. By using V Block method, we measured the refractive indices of LYSO in different directions. As shown in Fig. 5b, the LYSO:Ce sample for refractive index measurement was cut into the shape with right angles; faces (1) and (2) are perpendicular to faces (002) and (200) respectively. In monoclinic structures, which LYSO belongs to, crystals show distinct biaxial birefringence [32], and there are three principal refractive indices which are usually denoted as $N_g$, $N_m$, and $N_p$. As expressed in Fig. 5a, LYSO turns a beam of

---

![Figure 4](image-url) **Figure 4** Maps of rocking curve FWHM: (a) (200) face; (b) (020) face; (c) (002) face.

![Figure 5](image-url) **Figure 5** (a) The setup used to measure refractive index. (b) LYSO sample for refractive index measurement. (c) Directions in which the refractive indices of LYSO:Ce were measured.
incident ordinary light into two beams of extraordinary light; the bigger refractive index corresponds to $N_g$ and the other one corresponds to $N_p$. Their relation can be expressed as $N_g > N'_g > N_m > N'_p > N_p$. The measured refractive indices are plotted against wavelength and shown in Fig. 6. We found that our values of the refractive indices are close to those published in other papers [33, 34].

As we know that extraordinary light is anisotropic, its refractive index varies with directions. The measured refractive indices shown in Fig. 6 prove that there are indeed refractive index ($N'_g$ or $N'_p$) differences at every wavelength in different directions. Nevertheless, the refractive index differences in different directions are not more than 0.02. Therefore, we consider the anisotropy of refractive index as insignificant.

3.4 Anisotropy in transmittance By using the above-mentioned refractive indices, we also calculated the theoretical limit of transmittance according to Eq. (1), which is further deduced from Ref. [35] based on the hypothesis that the refractive index of air equals 1:

$$T(\lambda) = \frac{2n(\lambda)}{n^2(\lambda) + 1}. \quad (1)$$

We found that the differences of theoretical limit of transmittance between different directions are less than 0.27%, which is insignificant due to close values of refractive index.

The measured transmittance spectra show that in the directions perpendicular to planes (200), (020), and (002), all the transmittance at wavelength 404.7, 435.8, 486.1, 587.6, and 656.3 nm reaches their theoretical limit respectively, especially for the samples with a thickness of 2 mm (Fig. 7), showing that the LYSO crystal samples have high optical quality.

Figure 7b shows that the difference between any two measured transmittance spectra at 500 nm is not more than 0.3%. The difference is so small that it is even close to $\pm 0.1\%$, the photometric’s reproducibility. By comparing the transmittance spectra of LYSO crystal shown in Fig. 7, we found that the transmittance spectra were almost the same in the three directions (perpendicular to planes (200), (020), and (002), respectively) in the wavelength range of 200–800 nm, no matter whether the thickness of the samples is 2 or 16 mm. In a word, both calculated theoretical limit of transmittance and measured transmittance tend to support the insignificance of the transmittance anisotropy.

Since optical isotropy is one of the key requirements for a ceramic scintillator [36], the insignificance of anisotropy in transmittance and refractive index points out the potentiality of LYSO to be prepared in the form of optical ceramics. In fact, the ceramic LSO:Ce sample has shown high transparency and light yield value as high as 86% of that of good LSO:Ce crystal [37].

3.5 Anisotropy in luminescence mechanism It is well known that LSO:Ce and LYSO:Ce have two luminescence centers: Ce1 (7-oxygen-coordinated) and Ce2 (6-oxygen-coordinated) [38, 39]. To investigate the possible anisotropy in luminescence mechanism, UV excitation, and emission spectra of Ce1 and Ce2 were measured respectively. Fluorescence decay times of LYSO:Ce were also investigated. Given that the excitation spectra of the luminescence centers Ce1 and Ce2 in LYSO:Ce show...
overlap, in order to separate the excitation spectra of Ce1 apart from that of Ce2 as clearly as possible, we use 550 nm (much longer than the usually used 480–500 nm [38, 40–42]) as the monitoring emission wavelength for Ce2 luminescence centers. In this way, we reduce the overlap effect with Ce1 centers.

The results presented in Fig. 8 show that the peak profiles of excitation and emission spectra of crystal planes (200), (020), and (002) of LYSO:Ce are similar; the decay times are almost the same in these three different directions. Consequently, the anisotropy in the luminescence mechanism of LYSO:Ce is also insignificant.

### 3.6 Anisotropy in light output
We measured L.O. of the same LYSO:Ce sample by using its three different crystallographic surfaces as the coupled surface, respectively. As shown in Fig. 9, repeated tests show that the L.O. obtained with (020) as the coupled surface is lower (∼7%) than that obtained with (200) or (002) as the coupled surface, and the L.O. obtained respectively with (002), (200) as the coupled surface is close.

Given all of the factors listed below, the difference in the L.O. cannot be neglected and should be attributed to the anisotropy: (i) The systematic uncertainty of L.O. measurements in this work is ±1.7%, and the L.O. difference 7% is larger than two times the uncertainty. (ii) The sample for the L.O. measurements is the same, so there is no need to consider the potential contributing factor of Cerium concentration difference. (iii) The areas of the surfaces used for coupling to PMT were the same (297 mm²); the thicknesses in directions vertical to these three faces were also the same (16 mm). Hence, these potential contributing factors may also be neglected.

Figure 8 UV excitation spectra (a) Ce1: $\lambda_{\text{em}} = 404$ nm, (b) Ce2: $\lambda_{\text{em}} = 550$ nm and emission spectra (c) Ce1: $\lambda_{\text{ex}} = 348$ nm, (d) Ce2: $\lambda_{\text{ex}} = 327$ nm of LYSO:Ce crystal in the (200), (020), and (002) planes. (e) The fluorescence decay curves of LYSO:Ce crystal ($\lambda_{\text{ex}} = 348$ nm, $\lambda_{\text{em}} = 404$ nm) in the (200), (020), and (002) planes.

Figure 9 $^{137}$Cs pulse-height spectra of the same LYSO:Ce crystal sample coupled to PMT with (200), (020), and (002) crystal surfaces, respectively; the peak position indicating position of 662-keV line. The areas of these three faces being the same as 297 mm²; the thicknesses in directions vertical to these three faces were also the same (16 mm). Hence, these potential contributing factors may also be neglected.
3.7 Anisotropy in afterglow and thermoluminescence

Since afterglow decreases scintillation performance in nuclear medical imaging applications, it has always been a research hotspot from early times of LSO/LYSO study [43–48]. Afterglow curves of oriented LYSO:Ce crystal samples were measured and are shown in Fig. 10. The afterglow integrals in 0–0.25 and 0.25–2 ms were calculated and are listed in Table 2. It is clear that the afterglow intensity of plane (200) is lower than that of planes (020) and (002). We found that the relative afterglow intensity ratio of plane (200), (020), and (002) remains almost the same (78 ± 2%:100%:95%) in 0.25–2 ms.

However, no statement can be made at t ≥ 2 ms due to weak signal intensity and poor signal-to-noise ratio.

Thermoluminescence (TL) curves and also the wavelength resolved TL spectra were measured and are shown in Fig. 11. We found the spectrum shape and glow curve peak positions are the same in all three directions. This indicates the electron trap depth is the same in these three directions. As clearly shown in (a) and the contour line diagrams of 3D TL (b–d) in Fig. 11, the TL intensity of plane (200) is the weakest. By calculating the TL area (integral intensity) of planes (200), (020), and (002) in the temperature range 20–250 °C, we found the relative TL intensity ratio is 56%:100%:95% ((200):(020):(002)).

According to the results mentioned above, (200) plane has the weakest intensity both in TL and in afterglow, while (020) plane has the stronger intensity both in TL and in afterglow. Since traps addressed by above RT TL are responsible for afterglow phenomena in LSO and LYSO [43–55], the correlation between afterglow and TL results in this study further corroborates such a relationship. Given that the samples for these qualitative comparative studies are of the same size, shape, and polishing quality, the lowest and the highest trap-related light output appears in the planes

<table>
<thead>
<tr>
<th>plane</th>
<th>I(t = 0–0.25 ms)</th>
<th>I(t = 0.25–2 ms)</th>
<th>I(t = 0–2 ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(200)</td>
<td>0.066 (83%)</td>
<td>0.054 (78%)</td>
<td>0.119 (80%)</td>
</tr>
<tr>
<td>(020)</td>
<td>0.079 (100%)</td>
<td>0.069 (100%)</td>
<td>0.148 (100%)</td>
</tr>
<tr>
<td>(002)</td>
<td>0.084 (106%)</td>
<td>0.066 (95%)</td>
<td>0.151 (102%)</td>
</tr>
</tbody>
</table>

Figure 10 Afterglow curves of (200), (020), and (002) crystal planes in LYSO. The small figure plotted in the upper right corner of this figure presenting a partial enlargement of these curves.

Figure 11 (a) TL curves of LYSO crystal planes (200), (020), and (002). Wavelength resolved TL spectrum of (b) (200) plane, (c) (020) plane, and (d) (002) plane.
(200) and (020), respectively. This may be the reason for the phenomenon, as depicted in Fig. 9, that LYSO:Ce has respectively a relative higher or lower L.O. when (200) or (020) is selected as the coupled surface.

3.8 Contributing factors to the origin of the anisotropy phenomena

We note that it has been established that oxygen vacancy is the basic constituting element in the formation of deep electron traps [43, 50] and that it is especially the Si-nonbonded oxygen (usually named O5) that is subject to oxygen leave [56]. In addition, the Lu-O distances are considered important to understand the effect of oxygen vacancies [50, 56]. In LSO structure, the Lu1-O5 distances are 2.16 and 2.343 Å, and the Lu2-O5 are respectively a relative higher or lower L.O. when (200) or (020), respectively. This may be the reason for the weaker bonding force in this plane. In other words, Si-nonbonded oxygen tends to scatter in the corresponding (020) plane. However, it is opposite for (200) plane.

By analyzing the LYSO crystal structure, we found there are eight Si-nonbonded oxygens in the unit cell of its structure. Figure 12 clearly shows that the Si-nonbonded oxygen is concentrated in [010] direction, while it is relatively dispersed in [100] and [001] directions.

The coordinate positions of the Si-nonbonded oxygens were listed in Table 3. By calculation, we found the average coordinate positions of these Si-nonbonded oxygens in directions [100], [010], and [001] were the same – 0.5, i.e., the average coordinate positions were located in the middle of axes a, b, and c, respectively. As we know, planes (200), (020), and (002), respectively pass through the middle points of axes a, b, and c. If we represent the definition of offset parameter \( \Delta_o \) of Si-nonbonded oxygen in the following Eq. (2), we can evaluate the offset degrees of Si-nonbonded oxygen against planes (200), (020), and (002) (the middle points of axes a, b, and c, respectively).

\[
\Delta_o = \frac{1}{n} \sum_{n=1}^{n} \left[ O_n - \langle O \rangle \right] \times P
\]

In the equation, \( O_n \) represents the coordinate position of Si-nonbonded oxygen: \( x/a \) for [100] direction; \( y/b \) for [010] direction; and \( z/c \) for [001] direction. \( \langle O \rangle \) represents the average coordinate position of Si-nonbonded oxygen. \( P \)

represents the cell parameters \( a, b, \) and \( c \). Since there are eight Si-nonbonded oxygens in unit cell, \( n \) equals 8.

The calculated offset parameters were listed in Table 3 and plotted in Fig. 12. The results show the offset parameters \( \Delta_o \) of Si-nonbonded oxygen against planes (200) and (020) are respectively the largest and smallest. The smallest \( \Delta_o \) of Si-nonbonded oxygen against (020) plane indicates that Si-nonbonded oxygen concentrates in a flat region close to (020) plane. In other words, Si-nonbonded oxygen tends to scatter in the corresponding (020) plane. However, it is opposite for (200) plane.

Such a preferential distribution of Si-nonbonded oxygen, the origin of oxygen vacancy, can easily provide a platform for directional light output of afterglow and TL phenomena described above (Figs. 9–11).

Besides, the relative areal ion density ratio of planes (200), (020), and (002) is 100%:55%:72% (see Section 3.1 and Fig. 13). The lowest areal ion density of (020) plane indicates the lowest chemical bonds density and the larger distance between ions in this plane, thus naturally leading to the weaker bonding force in this plane. The weaker bonding force in (020) plane further tends to make the bonds in this plane easily broken. Hence, more defects tend to be involved in this plane. This may also be one of the contributing factors to the strongest TL and afterglow intensity of (200) plane. Similarly, the highest areal ion density of (200) plane may also be one of the contributing factors to the highest L.O., the weakest defect-related TL and afterglow intensity of (200) plane (Fig. 13).

It should be noted, however, that anisotropy effects are determined both by “surface effect” and “bulk effect.” Such anisotropy as the one in areal ion density, offset degree of Si-nonbonded oxygen against planes, and also its related defects corresponds to “surface effect.” Defect-related TL and afterglow are dependent largely on “surface effect.” Their corresponding anisotropy tends to be more obvious for a thin sample with a larger surface. However, since scintillation light travels in all possible directions and can be scattered in the corresponding (020) plane. Therefore, a platform for directional light output of afterglow and TL phenomena described above (Figs. 9–11).

Table 3 Coordinate positions \( O_n \), average coordinate positions \( \langle O \rangle \) of Si-nonbonded oxygens in (Lu0.913Y0.087)2SiO5:Ce structure. And also the offset parameters \( \Delta_o \) of Si-nonbonded oxygen against planes (200), (020), and (002).

<table>
<thead>
<tr>
<th></th>
<th>( x/a )</th>
<th>( y/b )</th>
<th>( z/c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( O_n )</td>
<td>0.0177</td>
<td>0.4034</td>
<td>0.8975</td>
</tr>
<tr>
<td>0.0177</td>
<td>0.9566</td>
<td>0.3975</td>
<td></td>
</tr>
<tr>
<td>0.5177</td>
<td>0.9034</td>
<td>0.8975</td>
<td></td>
</tr>
<tr>
<td>0.4823</td>
<td>0.9034</td>
<td>0.6025</td>
<td></td>
</tr>
<tr>
<td>0.5177</td>
<td>0.9066</td>
<td>0.3975</td>
<td></td>
</tr>
<tr>
<td>0.4823</td>
<td>0.9066</td>
<td>0.1025</td>
<td></td>
</tr>
<tr>
<td>0.9823</td>
<td>0.4034</td>
<td>0.6025</td>
<td></td>
</tr>
<tr>
<td>0.9823</td>
<td>0.9566</td>
<td>0.1025</td>
<td></td>
</tr>
</tbody>
</table>

\( \Delta_o \) (Å)

<table>
<thead>
<tr>
<th></th>
<th>(200)</th>
<th>(020)</th>
<th>(002)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>6.6445</td>
<td>2.2831</td>
<td>3.4518</td>
</tr>
</tbody>
</table>

The cell parameters of (Lu0.913Y0.087)2SiO5:Ce are: \( a = 14.263(3) \) Å, \( b = 6.6346(12) \) Å, \( c = 10.2421(18) \) Å.
reflected for many times inside the crystal before reaching the photodector, L.O. is dependent largely on “bulk effect” especially for a thick sample. Plane-related anisotropy has little impact on such kind of performance. This may contribute to the phenomenon that the anisotropy in L.O. is relatively inconspicuous as compared with that of TL and afterglow. The direction perpendicular to (020) plane, the most obvious anisotropy direction found for L.O., may tilt toward the surfaces of an unoriented cubic LYSO crystal sample. In other words, relatively inconspicuous anisotropy in L.O., and tilt of (020) to the surfaces, combined with “bulk effect” naturally lead to the phenomenon that the light output is isotropic for an unoriented cubic LYSO crystal sample mentioned at the beginning of this paper. In short, the plane-dependent anisotropy in areal ion density and Si-nonbonded oxygen distribution can be ascribed to the microstructure characteristics of LYSO:Ce. This anisotropy is proposed to be responsible for the anisotropy in defect and deep electron trap distribution, which may contribute to the afterglow, TL, and L.O. anisotropy mentioned before. Incidentally, it has to be noted that L.O. difference sometimes cannot be directly ascribed to TL and afterglow difference; they are sometimes anti-correlated. However, they are self-consistent in this study. One of the reasons for this may lie in the fact that the sample status (the potential contributing factors, such as sample size, shape, polishing quality, and transmittance) is well under control in this study.

4 Conclusions Despite the low structural symmetry of LYSO:Ce, surprisingly, the results presented here show that there is insignificant anisotropy in most of the properties of LYSO:Ce crystal – structural integrity, refractive index, transmittance, and luminescence mechanism. Insignificant optical anisotropy is very favorable for crystal processing and application, and also favorable for the ceramic form of this material.

We do observe anisotropy in the fine-structure, and also in afterglow, thermoluminescence characteristics and light output of small size samples as well. To explain such observations, we suggest that the anisotropy, determined by microstructure characteristics, in areal ion density and Si-nonbonded oxygen distribution leads to the directional anisotropy in the defect and electron trap distribution.

Although scintillation light is practically unpolarized, and the anisotropy of most properties of LYSO:Ce is inconspicuous, as proved by this work, further research by using polarized light source, polarization filter, and polarization dependent photodector might bring us more detailed anisotropy information about this crystal.

Acknowledgements The authors would like to thank Prof. Linhong Weng in Fudan University, Dr. Junjiang Hu in Shanghai Institute of Optics and Fine Mechanics, CAS, Dr. Junfeng Chen, Ze Xiong, Zhang Chen, and Prof. Shaohua Wang, Xuechao Liu in Shanghai Institute of Ceramics, CAS for the help in the single crystal diffraction, refractive index data acquisition, UV excitation and emission spectra, atomic force microscopy, rocking curves, and Raman spectra measurements. This work was supported by the Natural Science Foundation of Shanghai (Grant No. 09ZR1435800; 12GA-25) and project of Sino-Czech collaboration funded by MEYS, KONTAKT II (no. LH12185) program at the Czech side.

References
[33] http://nature.berkeley.edu/classes/eps2/wisc/LS2c.html