Research Article

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Photoluminescence characteristics and energy transfer phenomena in Ce$^{3+}$-doped YVO$_4$ single crystal

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Abstract: The undoped YVO$_4$ and Ce$^{3+}$-doped YVO$_4$ single crystals have been successfully grown by the Czochralski method in a medium frequency induction furnace. The X-ray diffraction patterns testified that all samples exhibited the pure tetragonal YVO$_4$ crystalline phase without any parasitic phases. The optical properties of Ce$^{3+}$-doped YVO$_4$ single crystals with different doping concentrations were investigated via a combination of absorption, emission, and excitation spectra. Dependence of luminescence and absorption intensity on Ce$^{3+}$ doping concentration was discussed at different excitation wavelengths. The typical transitions of Ce$^{3+}$ ions and the unusual intrinsic luminescence phenomena of VO$_4^{3-}$ groups were observed and investigated in Ce$^{3+}$-doped YVO$_4$ crystals. More attention was paid to ascertaining the corresponding transition states, analyzing luminescent mechanism, and revealing the energy transfer from VO$_4^{3-}$ to Ce$^{3+}$ ions. In addition, the CIE chromaticity coordinates and correlated color temperature were calculated on a basis of emission spectra under different excitation wavelengths.

Keywords: Ce$^{3+}$ ions, charge transfer state, luminescence, CIE chromaticity coordinate, color temperature

1 Introduction

Yttrium orthovanadate (YVO$_4$) is a promising optical material because it has a broad transparency spectra ranging from visible to far-infrared regions (400–5,000 nm), strong birefringence that ensures the polarization state of emitted light ($\Delta n = 0.2225$ for 633 nm), high damage threshold, high conductivity, good mechanical properties, and chemical stability [1–3]. The pure YVO$_4$ single crystal has been widely used as polarizers, optical isolators, and beam displacers [4–9]. As a good host for a variety of optical applications, rare-earth (RE)-doped YVO$_4$ materials have attracted significant attention. Owing to potential technological applications in the fields of display phosphors, laser materials, and fluorescent lamps, many researchers pay more attention to investigating the structural, magnetic, optical, and other properties of the YVO$_4$ doped with different rare-earth elements. For example, the Eu$^{3+}$-activated YVO$_4$ powder synthesized by the solid-state reaction, solution combustion, sol-gel, and the sonochemical method suggests high-efficiency fluorescence signal and higher thermal stability on electron-beam excitation so that it has been considered as an important commercial red phosphor used in cathode ray tube, fluorescent lamps, plasma display panels, and scintillator in image detectors [10–13]. The YVO$_4$ doped with Nd$^{3+}$ ions single crystal is an excellent laser material. Due to its low pumping threshold, large emission section, large absorption coefficient, strongly polarized laser output, and low susceptibility to electron irradiation, the Nd$^{3+}$-doped YVO$_4$ single crystal has been widely used in the diode-pumped solid lasers and self-frequency-doubling solid lasers [14–17]. In addition, Er$^{3+}$-doped YVO$_4$ and Yb$^{3+}$-doped YVO$_4$ crystals are very attractive potential directly diode-pumped laser materials with emission around 1.0 and 1.53$\mu$m [18]. The Tm$^{3+}$/Ho$^{3+}$/Er$^{3+}$/Yb$^{3+}$ co-doped YVO$_4$ phosphors exhibit bright white up-conversion emission upon 980 nm near-infrared excitation, which is a promising material for white light-emitting diodes [19].
The structural properties, elastic properties, hardness, and electronic structure of YVO₄ have been investigated extensively [3,20–22]. The YVO₄ belongs to the tetragonal crystallographic system (zircon-type phase) with space group $D_{4h}^{19}−I4_1/amd$ and lattice parameters $a = b = 0.71192$ nm, $c = 0.62898$ nm, and $a = \beta = \gamma = 90°$ [23]. The experimental and calculated theoretical band gaps $E_g$ are 3.7 and 3.0 eV, respectively [3,24,25]. The central metal ion $V^{5+}$ in isolated $VO_4^{−}$ group is coordinated by four oxygen ions in a tetrahedral symmetry [26]. The maximum phonon energy attributed to the totally symmetrical vibration ($A_{1g}$) in YVO₄ is about 890 cm$^{-1}$ [13]. The primitive unit cell of the YVO₄ single crystal contains four molecules of YVO₄ and RE$^{3+}$ ions occupy the Y$^{3+}$ lattice sites.

Up to now, the growth and spectral properties of RE$^{3+}$-doped YVO₄ (RE = Nd, Eu, Er, Tm, and Yb) phosphors and crystals have been reported extensively in the literature. In this paper, we focus on the photoluminescence properties and energy transfer phenomena in the Ce$^{3+}$-doped YVO₄ single crystal via a combination of absorption, excitation, and emission spectroscopy. More attentions were paid to ascertaining the corresponding transition states, analyzing luminescent mechanism, and revealing the energy transfer from $VO_4^{−}$ to Ce$^{3+}$ ions. Meanwhile, the concentration effect on the spectral properties is also investigated (the Ce$^{3+}$ doping concentration varies from $x = 0.005$ to $x = 0.06$ in YVO₄).

### 2 Experimental procedures

Pure YVO₄ and Ce$^{3+}$-doped YVO₄ crystals were grown by the Czochralski method in a medium frequency induction furnace. High-purity synthesized powders (>99.99%) of commercially available $Y_2O_3$, $V_2O_5$, and $Ce_2CO_3$ were applied to crystal growth. These raw materials were weighed and mixed in stoichiometric amounts. It is to be noticed that the CeO$_2$ is unstable at room temperature. Generally, the CeO$_2$ is used as a raw material of Ce$^{3+}$-doped optical crystals in reducing atmosphere. Nevertheless, it cannot rule out the possibility of some Ce$^{6+}$ ions existing in crystals. In this work, the Ce$_2(CO_3)_3$ is used to grow the Ce$^{3+}$-doped YVO₄ crystals in nitrogen atmosphere, which is considered as the donor of Ce$^{3+}$ ions. We believe that the reaction obeys the following equations:

$$\text{Ce}_2(CO_3)_3 \rightarrow \text{Ce}_2O_3 + 3CO_2 \uparrow (900°C)$$

$$xCeO_3 + yV_2O_5 + (1-x)Y_2O_3 \rightarrow 2Y_{1-x}Ce_xVO_4$$

The concentrations of Ce$^{3+}$ ions in YVO₄ single crystal vary from $x = 0.005$ to $x = 0.06$. The process of crystal growth has been reported in our previous work [27].

The X-ray diffraction (XRD) was measured at room temperature and performed by a Rigaku D/max 2500 v/PC diffractometer in the 2θ range from 10° to 90° in a step scan mode, with steps of 0.02°, using CuKα radiation of wavelength 0.154056 nm (40 kW/200 mA).

Absorption spectra were measured by a Shimadzu UV-3101 PC Spectrometer in the ultraviolet-visible and near infrared ranges (200–3,000 nm). The emission and excitation spectra were recorded with the Jobin-Yvon FL3221 TCSPC spectrophotometer and SPEX F-212 fluorescence spectrometer. Photoluminescence photographs were taken with Kimmon Koha IK Series Helium Cadmium 325 nm (He–Cd) laser systems in the darkroom. All tested samples are slices cutting from Ce$^{3+}$-doped YVO₄ single crystals with different Ce$^{3+}$ doping concentrations. The thickness of these slices is 2.00 mm after optically polishing. All the measurements were carried out at room temperature.

We did not carry out the X-ray fluorescence (XRF) measurement so that the actual Ce$^{3+}$ doping concentrations in the Ce$^{3+}$-doped YVO₄ crystals are not obtained through the XRF. The final heat treatment and annealing process have an effect on the photoluminescence, but don’t affect the luminescent mechanism. In addition, the segregation phenomenon also leads to the difference between actual cerium ion concentration and theoretical concentration in different parts of the as-grown crystal. Therefore, the theoretical calculations of optical parameters related to Ce$^{3+}$ doping concentration are not carried out in this paper, such as absorption cross, integrated absorption cross, integrated emission cross-section, energy transfer probability, critical distance, and so on.

### 3 Results and discussion

Figure 1(a) and (b) show the photographs of as-grown undoped YVO₄ single crystals and Ce$^{3+}$-doped YVO₄ single crystals with various cerium doping concentrations, respectively. The test specimens are Ce$^{3+}$-doped YVO₄ single-crystal slices, as shown in Figure 1(c). The XRD patterns of the pure YVO₄ and Ce$^{3+}$-doped YVO₄ crystals are presented in Figure 2. The strong XRD peaks are collected in a wide angle range and some evident peaks are assigned. The diffraction peaks and relative intensity agree well with the standard data of YVO₄ (JCPDS card No. 72-0341), which indicates that the obtained phase is YVO₄.
without any parasitic phase, such as the Y_2O_3 or V_2O_5 phases. The Ce^{3+} ions enter into the YVO_4 crystal and occupy the Y^{3+} lattice sites. The ionic radii of Ce^{3+} and Y^{3+} ions are 0.102 and 0.1015 nm [28–30], respectively. It is obvious that the radius of Ce^{3+} ions is very similar to that of the Y^{3+} ions so that the lattice distortion caused by Ce^{3+} ions is very small, which contributes to the crystal growth. However, the higher Ce^{3+} ions are doped in the crystal, the more severe lattice distortion is. The samples doped with different Ce^{3+} concentrations exhibit the pure tetragonal YVO_4 crystalline phase. It is indicated that partial substitution of Ce^{3+} for Y^{3+} does not affect the structure of YVO_4 phase and the Ce^{3+} ions doped into the host lattice effectively [31].

For a free Ce^{3+} ion, its electronic configuration is 4f^1. The free-ion Hamiltonian (including electron-electron and spin-orbit interaction terms) produces the 2S+1L_J multiplets. We only consider the spin-orbit coupling of trivalent rare earth and do not take account of Stark splitting under the influence of the crystal field. Based

Figure 1: Photographs of as-grown YVO_4 and Ce^{3+}-doped YVO_4 single crystal. (a) Pure YVO_4 single crystals, (b) Ce^{3+}-doped YVO_4 single crystals with different doping concentrations, (c) Ce^{3+}-doped YVO_4 single-crystal slices (the Ce^{3+} doping concentrations vary from \( x = 0.005 \) to \( x = 0.06 \). The thickness of these slices is 2.00 mm after optical polishing).
on the Hund’s rules, the ground state is $^2F_{5/2}$ and the excited state is $^2F_{7/2}$. The energy gap between $^2F_{7/2}$ and $^2F_{5/2}$ states is about $2,200 \text{ cm}^{-1}$ [27,32,33]. The 5d energy levels of the excited 4f$_0$5d$_1$ configuration form a 2D term splitting into $^2D_{3/2}$ and $^2D_{5/2}$ states, which are influenced strongly by the crystal field of the host. The energy gap between $^2D_{3/2}$ and $^2D_{5/2}$ states is about $1,890 \text{ cm}^{-1}$ [34,35]. The energy of the 5d levels is so low that the spectra of 5d–4f transition can be observed in the near-ultraviolet and visible ranges.

Figure 3 shows the absorption spectra of pure YVO$_4$ and Ce$^{3+}$-doped YVO$_4$ crystals in the ultraviolet-visible and near infrared ranges at room temperature. The pure YVO$_4$ crystal exhibits a very wide transparency spectrum ranging from 500 to 3,000 nm, while an intense broad absorption bands below 350 nm can be recorded. The same intense absorption bands below 350 nm are also observed in the samples with different dopant concentrations. Up to now, this phenomenon has been well-understood. The central metal ion V$^{5+}$ in isolated VO$_4^{3-}$ group is coordinated by four oxygen ions in a tetrahedral symmetry [31,36]. The theoretical studies have proven that the molecular orbital of V$^{5+}$ ion in isolated VO$_4^{3-}$ group gives rise to a $^1A_g$ ground state with configuration $t_{2g}^6e_{g}^0$ and four excited states with configuration $t_{2g}^1e_{g}^1$, which are $^3T_1$, $^3T_2$, $^1T_1$, and $^1T_2$, respectively [37–39]. Therefore, the intense absorption band below 350 nm is ascribed to the intrinsic absorption of VO$_4^{3-}$, which is the charge transfer absorption transitions from the $^1A_g$ ground state to the $^3T_1$, $^3T_2$, $^1T_1$, and $^1T_2$ excited states. Compared with pure YVO$_4$ single crystal, the YVO$_4$ crystals with Ce$^{3+}$ doping concentration of $x = 0.005$, $0.01$, $0.02$, $0.05$ exhibit the broad absorption band (centered at 460 nm) ranging from 380 to 880 nm. Moreover, the absorption becomes stronger and stronger with increasing the Ce$^{3+}$ doping concentration. The Ce$^{3+}$ doping concentration of $x = 0.06$ leads to the whole absorption below 640 nm. It is obvious that the absorption band is associated with typical transition of the Ce$^{3+}$ ions, which are assigned to the superposition of the $^2F_{5/2} \rightarrow ^2D_{3/2}$ and $^2F_{5/2} \rightarrow ^2D_{5/2}$ absorption transitions. Broader absorption band and larger absorption cross-section serve to absorb the pump light and improve the conversion efficiency of pump light [40].

Figure 4 shows the visible emission spectra of Ce$^{3+}$-doped YVO$_4$ crystals with different cerium doping concentrations (from $x = 0.005$ to $x = 0.06$). On a basis of the absorption spectrum (Figure 3), the excitation wavelength at 460 nm is applied to pumping all the samples. As can be seen from the Figure 4, a very broad emission band centered at about 620 nm is observed in the region from 480 to 800 nm. Except for the emission intensity, the obtained spectra are identical in the range of 480–800 nm. The 460 nm excitation wavelength corresponds to the $^2F_{5/2} \rightarrow ^2D_{3/2}$ absorption transition of Ce$^{3+}$ ions. However, it is very difficult to determine the energy levels of emission transition. Wang et al. [41] studied the same broad emission band and concluded that the broad emission band centered at 620 nm was attributed to the charge transfer transition of the Ce$^{4+}$–O$^{2-}$ ions pairs (CTS$_2 \rightarrow$ CTS$_3$).
Generally speaking, the charge transfer transition of rare-earth ions is usually located in the ultraviolet range, such as Lu2Si2O7:Ce3+ [42,43], YVO4:Eu3+ [13,44,45], Na2YMg2(VO4)3:Yb3+ [31,46]. The red emission band at 620 nm corresponding to the 3T1 → 1A1 transition has been also observed in the pure Zn3(VO4)2, Ca5Mg4(VO4)6, Ca5Zn4(VO4)6, and NaYMg2(VO4)3 single crystals with isolated VO4 tetrahedra [26,31,47]. Moreover, the influences of phonons and Stark split induced by crystal field cannot be neglected. In the view of above analysis, we assume that the observed broad band centered at about 620 nm can be assigned to the 3T1 → 1A1 transition (the charge transfer from oxygen ligands to the central vanadium atom inside the VO4−). On the other hand, it can be also assigned to the 2D3/2 → 2F7/2 transition under the joint action of the phonons and crystal filed. Thus, it can be concluded that the broad is attributed to the overlap of the 3T1 → 1A1 transition and phonon-assisted 2D3/2 → 2F7/2 transition under the influence of ligand field.

Since the radial wave function of the excited 5d electron extends spatially well beyond the closed 5s25p6 shells, the 2D3/2 and 2D5/2 states are strongly perturbed by the ligand field of the host. The absorption and emission wavelength of Ce3+-doped different oxides have been published in ref. [35]. These data are listed in Table 1. The different hosts lead to a great change in the f–d transition, which is different from the f–f transition of 4f electronic configuration.

In order to investigate the spectral properties and analyze the energy transfer mechanism from VO4− (the host) to Ce3+ ions, the emission spectra of Ce3+-doped YVO4 crystals with various dopant concentrations from

![Figure 4: Visible emission spectra of Ce3+-doped YVO4 crystals with various doping concentrations. The excitation wavelength is 460 nm corresponding to the 2F5/2 → 2D3/2 absorption transition of Ce3+ ions.](image)

![Figure 5: Emission spectra of Ce3+-doped YVO4 crystals with different cerium doping concentrations. The excitation wavelength is 325 nm corresponding to the 1A1 → 1T2 absorption transition of VO4−.](image)

### Table 1: Absorption and emission wavelength of Ce3+-doped different oxides

<table>
<thead>
<tr>
<th>Host</th>
<th>Absorption wavelength λabs (nm)</th>
<th>Emission wavelength λem (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>YPO4</td>
<td>320</td>
<td>333</td>
</tr>
<tr>
<td>YAl3(BO3)4</td>
<td>322</td>
<td>338</td>
</tr>
<tr>
<td>YBO3</td>
<td>357</td>
<td>383</td>
</tr>
<tr>
<td>LiYSiO4</td>
<td>348</td>
<td>397</td>
</tr>
<tr>
<td>YAlO3</td>
<td>303</td>
<td>345</td>
</tr>
<tr>
<td>Y3Al1O12</td>
<td>458</td>
<td>535</td>
</tr>
<tr>
<td>Y3Al4GaO12</td>
<td>445</td>
<td>523</td>
</tr>
<tr>
<td>Sr2Y2O4</td>
<td>397</td>
<td>560</td>
</tr>
<tr>
<td>YVO4*</td>
<td>460</td>
<td>620</td>
</tr>
</tbody>
</table>

*Present work.

\[ x = 0.005 \text{ to } 0.6 \] were measured at room temperature, as shown in Figure 5. The excitation wavelength was chosen to be 325 nm corresponding to the 1A1 → 1T2 absorption transition of VO4−. Besides the broad emission bands centered at 440 nm from 350 to 600 nm for all samples showing up obviously, a weak emission band centered at 620 nm was also recorded. Except for the emission intensity, all obtained spectra are identical in the range of 350–750 nm. It is well-known that the energy transfer from VO4− to the doped rare-earth ions is so efficient that the intrinsic luminescence of the host cannot be observed at room temperature. Although some literatures have reported the intrinsic emission of VO4− in the rare-earth-doped YVO4 materials at room temperature, the doping concentration of rare-earth ions is very low (less than
When the doping concentration reaches more than \( x = 0.01 \), the intrinsic luminescence tends to disappear in the emission spectra. Therefore, we believe that the broad emission band centered at 440 nm from 350 to 600 nm must be attributed to the luminescence of the Ce\(^{3+}\) ions, which is the overlap of the \( ^2D_{3/2} \rightarrow ^2F_{7/2} \) (P\(_2\) centered at 470 nm) and \( ^2D_{3/2} \rightarrow ^2F_{5/2} \) (P\(_1\) centered at 428 nm) emission transitions. Figure 6 shows the fitting curves of the emission spectra. The luminescent photographs of the Ce\(^{3+}\)-doped YVO\(_4\) single crystals excited at 325 nm are shown in Figure 7, which are taken in darkroom. Intense blue emissions are observed at room temperature. According to the fitting data, the energy gap between the \( ^2F_{7/2} \) and \( ^2F_{5/2} \) states is about 2,088 cm\(^{-1}\), which is in good agreement with theoretical values 2,200 cm\(^{-1}\) [27,32,33]. As can be seen from Figure 5, a narrow emission band centered 620 nm appears in the emission spectra excited at 325 nm, which is also observed in other pure undoped single crystals with isolated VO\(_4^\text{-}\) (act as a luminescent center) tetrahedra [26,31,46,47]. According to the energy level of VO\(_4^\text{-}\) group in other materials, we can assume that the narrow emission band is assigned to the \( ^3T_{2} \rightarrow ^1A_{1} \) (620 nm) transitions. However, the intrinsic luminescence of the host in the highly Ce\(^{3+}\)-doped YVO\(_4\) crystal (more than \( x = 0.01 \)) is not acceptable. Zhou et al. [2] have investigated the unusual intrinsic luminescence of YVO\(_4\):Er\(^{3+}\) phosphors (dopant concentration \( x = 0.005, 0.02, 0.04, \) and 0.06). They believe that this phenomenon means very little amount of rare-earth ions successfully entered the host or the energy transfer between VO\(_4^\text{-}\) and rare-earth ions was not efficient. The analysis of the XRD patterns has proven that the obtained phase is YVO\(_4\) without any parasitic phase, such as the Y\(_2\)O\(_3\) or V\(_2\)O\(_5\) phases. Moreover, the radius of Ce\(^{3+}\) ions is very similar to that of the Y\(^{3+}\) ions so that the lattice distortion caused by Ce\(^{3+}\) ions is very small and the Y\(^{3+}\) lattice sites are occupied by the Ce\(^{3+}\) ions easily. In addition, the ref. [2,31] all reported that the intrinsic luminescence of the host could decrease with the doping concentration. The Figure 5 displays the

![Figure 6: Gaussian fitting curve of the emission spectra excited at 325 nm.](image)

![Figure 7: Luminescent photographs of the YVO\(_4\) (a) and Ce\(^{3+}\)-doped YVO\(_4\) single crystals excited at 325 nm (Doping concentration is \( x = 0.005 \) (b), 0.01 (c), 0.02 (d), 0.05 (e), and 0.06 (f), respectively.](image)
opposite behavior, which suggests this narrow emission band may correspond to luminescence properties of the Ce$^{3+}$ ions. Moreover, if the 620 nm emission would arise from VO$_4^{3-}$, it should be a very broad band [52]. This emission band is very sharp and weak so that it also looks like the transition from the 5D(0) state to the $7F(J)(J = 0, 1, 2, 3, 4)$ states of unintentionally contaminated Eu$^{3+}$ ions. But all the experimental specimens with various Ce$^{3+}$ doping concentrations show the same characterization, which basically rules out the possibility of the unintentionally contaminated Eu$^{3+}$ ions. This phenomenon always puzzles us and the reason why the intrinsic emission appears in the emission spectra needs further study.

Figure 8 shows the excitation spectra of Ce$^{3+}$-doped YVO$_4$ single crystal for 620 nm (a), 440 nm (b), and 470 nm (c) emissions at room temperature. Monitoring the emissions at 620, 440, and 470 nm, the specimen exhibits a broad excitation band extending from 260 to 360 nm, which is attributed to the $1A_1 \rightarrow 1T_2$, $1T_1$ charge transfer band (CT) of V$^{5+}$–O$^{2-}$ (from oxygen ligands to the central vanadium atom inside VO$_4^{3-}$ groups in the YVO$_4$) [53–55]. Under excitation of UV lights (260–360 nm), the emission intensities of 440 and 470 nm are stronger than those of 620 nm. This result is consistent with analysis of photoluminescence emission spectra (Figure 5). Differing from Figure 8(b) and (c), a strong excitation band located at about 565 nm and two weak excitation bands at 395 and 460 nm are recorded in Figure 8(a). The two weak excitation bands are associated with typical transitions of the Ce$^{3+}$ ions, which are assigned to the $^2F_{5/2} \rightarrow ^2D_{5/2}$ (395 nm) and $^2F_{5/2} \rightarrow ^2D_{3/2}$ (460 nm) transitions, respectively. The observed strong excitation band at 565 nm could be assigned to the charge transfer transition between V$^{5+}$ and O$^{2-}$, described as $^1A_1 \rightarrow ^3T_2$, $^3T_1$ transition. Compared to the typical excitation bands of the Ce$^{3+}$ ions, the charge transfer band is more suitable for 620 nm emission. The excitation spectra displaying a strong charge transfer band means that the host (VO$_4^{3-}$ group) can absorb the pump energy (UV-photon) intensively and then transfer the energy to the nearby Ce$^{3+}$ ions efficiently. This process can improve the conversion efficiency of the pump light and promote the luminescent properties of rare-earth ions.

![Figure 8](image-url)

**Figure 8**: Excitation spectra of Ce$^{3+}$-doped YVO$_4$ single crystal for 620 nm (a), 440 nm (b), and 470 nm (c) emissions at room temperature.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Concentration</th>
<th>Excitation wavelength (nm)</th>
<th>Calculation data ranges from $\lambda_1$ to $\lambda_2$ (nm)</th>
<th>CIE chromaticity coordinates</th>
<th>Color</th>
<th>Color temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y$_{1-x}$Ce$_x$VO$_4$ single crystal</td>
<td>$x = 0.005$</td>
<td>325</td>
<td>355–700</td>
<td>0.1649 0.1458</td>
<td>Blue</td>
<td>7836.454</td>
</tr>
<tr>
<td></td>
<td>460</td>
<td>480–800</td>
<td>0.4974 0.4875</td>
<td>Yellow</td>
<td>2763.211</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$x = 0.01$</td>
<td>325</td>
<td>355–700</td>
<td>0.1655 0.1485</td>
<td>Blue</td>
<td>7771.629</td>
</tr>
<tr>
<td></td>
<td>460</td>
<td>480–800</td>
<td>0.5006 0.4849</td>
<td>Yellow</td>
<td>2712.763</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$x = 0.02$</td>
<td>325</td>
<td>355–700</td>
<td>0.1666 0.1565</td>
<td>Blue</td>
<td>2923.931</td>
</tr>
<tr>
<td></td>
<td>460</td>
<td>480–800</td>
<td>0.4941 0.4903</td>
<td>Yellow</td>
<td>2816.445</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$x = 0.05$</td>
<td>325</td>
<td>355–700</td>
<td>0.1653 0.1514</td>
<td>Blue</td>
<td>7099.445</td>
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<tr>
<td></td>
<td>460</td>
<td>480–800</td>
<td>0.4943 0.4902</td>
<td>Yellow</td>
<td>2813.62</td>
<td></td>
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<tr>
<td></td>
<td>$x = 0.06$</td>
<td>325</td>
<td>355–700</td>
<td>0.1697 0.1562</td>
<td>Blue</td>
<td>4118.842</td>
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<tr>
<td></td>
<td>460</td>
<td>480–800</td>
<td>0.4966 0.4882</td>
<td>Yellow</td>
<td>2776.2</td>
<td></td>
</tr>
</tbody>
</table>
The CIE coordinates and correlated color temperatures (CCTs) are two important characteristics for luminous materials [56]. The color coordinates can be obtained on a basis of emission spectra (Figures 4 and 5). According to the CIE chromaticity coordinate, the correlated color temperature also can be calculated through the following approximate formula proposed by McCamy [19,57–59].

\[
\text{CCT}(x, y) = -437n^3 + 3,601n^2 - 6,861n + 5514.31 \tag{3}
\]

where \( n = (x - x_e)/(y - y_e) \) is the inverse slope line, and \( x_e = 0.3320, y_e = 0.1858 \).

The CIE chromaticity coordinates and correlated color temperatures of Ce\(^{3+}\)-doped YVO\(_4\) crystals have been calculated under different excitation wavelengths, as listed in Table 2. Figure 9 presents the CIE chromaticity coordinates \((x, y)\) positions of Ce\(^{3+}\)-doped YVO\(_4\) single crystals in the Commission Internationale de l’Eclairage (CIE) 1931 chromaticity diagram. It is clear that the samples excited at 325 nm are located in blue region, which is in good agreement with Figure 7. When the excitation wavelength is 460 nm, the samples are located in yellow region. In addition, the Ce\(^{3+}\) doping concentration has little effect on the emitting color.

4 Conclusion

In summary, the high-quality YVO\(_4\) and Ce\(^{3+}\)-doped YVO\(_4\) single crystals were grown by the Czochralski method. The X-ray diffraction (XRD) patterns indicated that the obtained phase was YVO\(_4\) without any parasitic phase. Optical properties of Ce\(^{3+}\)-doped YVO\(_4\) single crystal with different doping concentrations were investigated via a combination of absorption, excitation, and emission spectra. Particularly, more attentions were paid to ascertaining the corresponding transition states, analyzing the luminescence mechanism and revealing the charge transfer (CT) transition in Ce\(^{3+}\)-doped YVO\(_4\) single crystals. Based on the experimental data, CIE chromaticity coordinates and correlated color temperatures of Ce\(^{3+}\)-doped YVO\(_4\) crystals were calculated and depicted in CIE chromaticity diagram.

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