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Scintillation Properties of $KCu_2I_3 \cdot CH_3SOCH_3$ and $RbCu_2I_3 \cdot CH_3SOCH_3$ Single Crystals

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$KCu_2I_3 \cdot$DMSO (K sample, DMSO: dimethyl sulfoxide) and $RbCu_2I_3 \cdot$DMSO (Rb sample) single crystals were fabricated by the solvent diffusion method. The K and Rb samples exhibited a broad emission band peaking at 550 and 530 nm, respectively, in the photoluminescence (PL) spectra. The PL quantum yield values under 450 nm excitation were 26 and 55% for the K and Rb samples, and the decay time constants were calculated to be 1.96 and 1.93 µs, respectively. These emissions were attributed to the cluster-centered charge transfer transitions. The X-ray-induced radioluminescence spectra were almost consistent with the PL spectra; thus, the emissions can be assigned to the same origin. The light yields of the K and Rb samples were estimated to be approximately 2800 and 2600 photons/MeV under γ-ray exposure, respectively.

1. Introduction

Scintillators play a crucial role in the detection of ionizing radiation, such as X- and γ-rays, by immediately converting high-energy radiation into UV–NIR light, which can be measured with photodetectors. They are widely employed in scintillation detectors for radiation monitoring, such as medical diagnosis,(1–3) security inspections,(4–6) astrophysics research,(7–9) and high-energy physics experiments.(10–12) These materials have been developed in various forms,(13–15) including single crystals,(16–20) glasses,(21–25) and ceramics.(26–30) Among them, single crystals are considered the most primary class of scintillators owing to their high transparency, high density, and high light yield (*LY*).(13,31,32) However, the synthesis of single crystals generally requires high-temperature melt-growth processes, which pose challenges in terms of high energy consumption and equipment costs. A promising alternative to address these limitations is the solution-growth method, which has recently attracted attention owing to its capability of synthesizing crystals at temperatures lower than those of conventional melt-growth processes.(33–35)

Organic–inorganic hybrid materials have attracted interest as a new class of scintillators that can be synthesized by low-temperature solution-growth methods.(36–38) Of these, low-

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dimensional CuI-based cluster compounds are considered promising materials for scintillators owing to their unique electronic structures and favorable luminescence properties.(39–41) These compounds offer the advantage of potentially achieving high photoluminescence (PL) quantum yield (*QY*), owing to quantum confinement effects associated with their low-dimensional structures. According to Robbins' theoretical formula, the scintillation *LY* is proportional to the PL *QY* of the emission center.(42) Therefore, high *QY* is one of the essential parameters for exhibiting good scintillation performance. In addition, their moderate Stokes shifts help mitigate *LY* loss caused by self-absorption.(43,44) Here, KCu_2I_3·dimethyl sulfoxide (DMSO) and $RbCu_2I_3$·DMSO, which have been reported as phosphors for LED applications, but yet to be studied in detail for radiation detection, were focused on.(45) Hereafter, KCu_2I_3·DMSO and $RbCu_2I_3$·DMSO are called K and Rb samples, respectively. These compounds are promising candidates for low-temperature solution processable scintillators because they can be synthesized at room temperature and exhibit emissions at around 535 nm with reported PL *QY* values of 27.5–38.2%. However, the scintillation performance under ionizing radiation has not been clarified. In this study, the CuI-based organic–inorganic hybrid single crystals were fabricated by the solvent diffusion method, and their PL and scintillation properties were evaluated to explore their potential as scintillators that combine high *LY* with low-temperature solution processability, toward future applications in simple and scalable radiation detector platforms.

2. Experimental Procedure

The crystals were synthesized by the solvent diffusion method. A precursor solution was prepared by dissolving 4 mmol of CuI (99.99%, High Purity Chemicals) and 2 mmol of either KI (99%, High Purity Chemicals) or RbI (99%, Mitsuwa Chemicals) in 2 mL of DMSO (99.5%, Fujifilm Wako Pure Chemical). To prevent the oxidation of Cu^+, 0.05 mL of phosphinic acid solution (50%, Fujifilm Wako Pure Chemical) was added. The crystals were obtained by diffusing 1 mL of chlorobenzene (Fujifilm Wako Pure Chemical) as a poor solvent into 0.1 mL of the precursor solution, kept at 30 °C to ensure consistent synthesis conditions, over several days.(45) The obtained crystals were used for measurements in the as-grown form. The PL and PL excitation (PLE) 3D spectra and the absolute PL *QY* were measured using a Quantaurus-QY spectrometer (Hamamatsu Photonics, C11347). PL decay time profiles (excitation wavelength: 405 nm, emission wavelength: 530 nm) were measured using a Quantaurus-τ spectrometer (Hamamatsu Photonics, C11367). X-ray-induced radioluminescence (XRL) spectra were measured using our original setup.(46) Pulse-height spectra (PHS) under ^{137}Cs γ-ray (662 keV) irradiation were measured with a shaping time of 6 μs, consisting of a photomultiplier tube (PMT, Hamamatsu Photonics, R7600U-200), amplifiers (Ortec, 113 and 570), and a multichannel analyzer (Amptek, Pocket MCA8000A).

3. Results and Discussion

Figure 1(a) shows the PL/PLE 3D spectra of the samples. The emission intensity was normalized to the highest signal intensity, and the scales of intensities are also shown. Broad emission bands peaking at 560 and 530 nm were observed for the K and Rb samples under excitation at 350–480 nm, corresponding to Stokes shifts of approximately 0.54 and 0.30 eV, respectively. The PL *QY*s under excitation at 450 nm were 26% for the K sample and 55% for the Rb sample. This difference in PL *QY* are related to structural distortions and variations in bond angles within the CuI clusters, induced by the difference in ionic radii between K^+ and Rb^+.(39) Figure 1(a) insets show the appearance of the samples and their emission under UV light (wavelength: 365 nm). Both samples were yellow crystals, approximately 2–3 mm in size, and exhibited a yellowish-green emission under UV excitation. The K sample exhibited rougher surfaces and more visible cracks than the Rb sample, suggesting that its overall crystal quality was lower. Figure 1(b) shows the PL decay time profiles of the samples. The decay curves were approximated with a single exponential decay model. The decay time constants were calculated to be 1.95 for the K sample and 1.93 μs for the Rb sample. Both samples exhibited similar spectral shapes and decay behaviors, suggesting that the emission originates from the same luminescent center. Since these decay time constants were close to the microsecond-order values reported in past studies of Cu-based cluster compounds, the emissions were attributed to cluster-centered (CC) charge transfer transitions.(45)

Figure 2(a) shows the XRL spectra of the samples. The emission bands were almost consistent with the PL spectra, and thus, they can be attributed to a similar origin. In both samples, a small

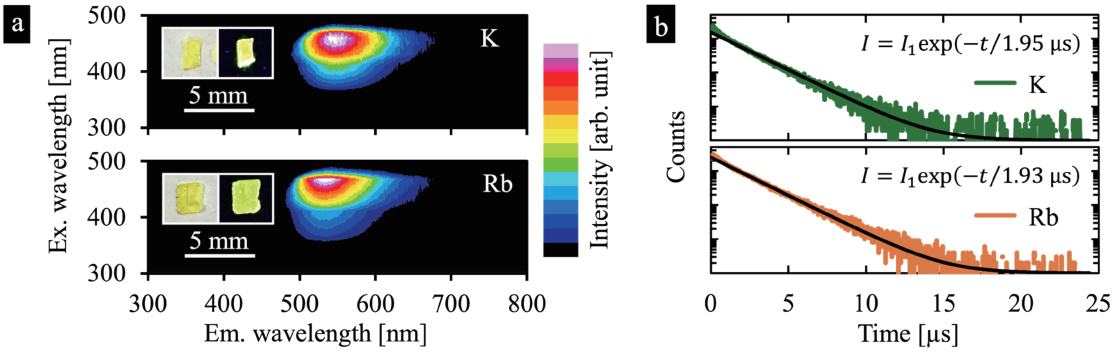

Fig. 1. (Color online) (a) PL/PLE 3D spectra. The insets show the appearance of samples under room light and UV light (λ = 365 nm). (b) PL decay time profiles of the K and Rb samples (λ_{ex} = 405 nm, λ_{em} = 530 nm).

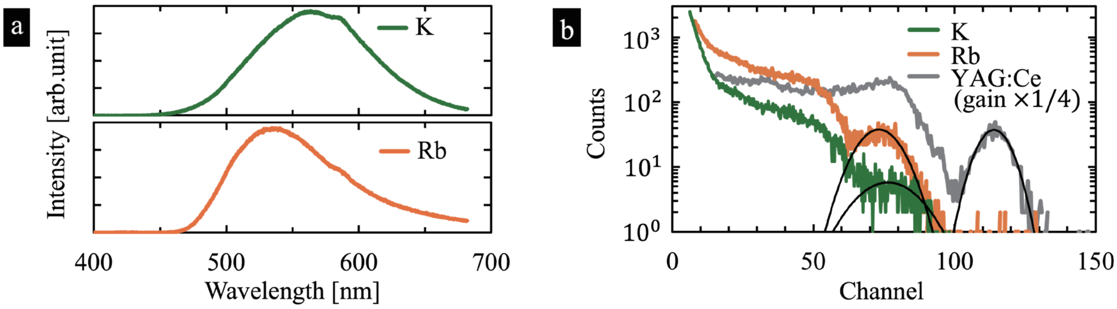

Fig. 2. (Color online) (a) X-ray-induced radioluminescence spectra, and (b) pulse-height spectra of the K and Rb samples.

peak was observed at around 590 nm, which was an instrumental artifact and not derived from the samples. Figure 2(b) shows the PHS of the samples and a reference Ce-doped $Y_3Al_5O_{12}$ (YAG:Ce) commercial scintillator (Konoshima Chemical, LY = 20000 photons/MeV). Photoabsorption peaks at 662 keV were observed for the K and Rb samples and the YAG:Ce at channels of 76, 73, and 456, respectively. The quantum efficiencies of the PMT at the emission wavelengths of the K and Rb samples and YAG:Ce were 9.4, 9.7 and 7.9%, respectively. On the basis of the comparison with the YAG:Ce reference, the LY values of the K and Rb samples were calculated to be approximately 2800 and 2600 photons/MeV, respectively. According to Robbins' simplified model, LY is expressed as $LY \propto S \cdot QY/E_g$, where S is the energy transfer efficiency, and E_g is the bandgap energy.(42,47) In this study, the E_g values of the K and Rb samples were assumed to be nearly identical, as both compounds share similar chemical compositions and structural motifs. Under this assumption, no significant difference in LY was observed, although the QY of the Rb sample was more than twice that of the K sample. The result suggests that the S of the Rb sample is inferior to that of the K sample, possibly because of the poor crystal quality of the K sample, such as the presence of cracks, which may reduce the efficiency of energy transfer from the host lattice to the luminescent centers.

4. Conclusions

In this study, K and Rb samples with a bulk single crystal form were synthesized via a low-temperature solvent diffusion method, and their PL and scintillation properties were evaluated. Both samples exhibited broad emission bands attributed to CC charge transfer transitions. The PL decay time constants were calculated to be 1.95 and 1.93 μs, respectively. The PHS revealed that the LY values of the K and Rb samples were estimated to be approximately 2800 and 2600 photons/MeV, respectively. These results demonstrate that CuI cluster-based hybrid single crystals synthesized at low temperatures exhibit measurable scintillation responses and have potential as novel scintillators. Furthermore, since the interaction between the CuI clusters and ligands affects both the crystal growth and the luminescence properties, tuning this interaction can lead to improved performance as a scintillator.

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