Relationship between crystal structure and luminescence properties for Ce^{3+}-doped rare-earth pyrosilicate

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Ce^{3+}-doped rare-earth (RE) pyrosilicate (Ce:$RE_2Si_2O_7$) have been reported as a scintillator capable of converting energy of ionizing radiation to ultra-violet or visible light [1,2]. The electric configuration of Ce^{3+} ion is defined to be [Xe]$4f^1$ and Ce^{3+} ion can be excited into [Xe]$4f^05d^1$ electronic configuration [3]. Since the 5d electron of Ce^{3+} ion is existed in the outermost-shell, degenerated 5d levels of Ce^{3+} ion splits due to both of the crystal field strength in Ce^{3+} site and the deviation of the electric charges in the crystal field of Ce^{3+} ion. Here, the crystal structures of Ce:$RE_2Si_2O_7$ have diverse range of crystal systems and space groups depending on the average RE ionic radii [4]. In this study, we performed a comprehensive study of Ce:$RE_2Si_2O_7$ to investigate the relationship between the crystal structure and the luminescence properties.

Since the most $RE_2Si_2O_7$ have incongruently melting compound and difficult to grow single crystals from the melt, we synthesized the sintered compacts using solid reaction method. As starting materials, commercial oxide powders (SiO_2, Y_2O_3, La_2O_3, CeO_2, Gd_2O_3 and Lu_2O_3) with purities of over 99.99% were used. After weighing according to $(Ce_{0.01}\ RE_{0.99})_2Si_2O_7$ (RE= La, Gd, Y and Lu), $(Ce_{0.01}\ RE_{0.50}\ RE'_{0.49})_2Si_2O_7$ ((RE,RE') = (La,Gd), (La,Y), (La,Lu), (Y, Gd), (Gd, Lu) and (Lu, Y)) and $(Ce_{0.01}\ Y_{0.24}\ Lu_{0.75})_2Si_2O_7$, the powders were formed into pellets by a hydraulic press. The pellets were pre-sintered at 1550°C for 12 hours under air atmosphere. After that, main sintering was performed at 1600°C for over 48 hours under air atmosphere.

The powder X-ray diffraction analysis results show that the phases of $(Gd,Lu)_2Si_2O_7$ and $(La,Lu)_2Si_2O_7$ are not single phase. On the other hand, the other samples were obtained single phase and classified into three kinds crystalline systems (*C*2/*m*, *Pna*2_1 and *P*2_1/*c*) according to the average RE ionic radii. The crystal structure information (lattice parameters and atomic coordinates) was identified by the Rietveld refinement technique, and it was found that the average RE-O bond lengths were increased as the average RE ionic radii were increased.

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