XRD and energy band studies of Eu³⁺ doped MgSiO3, SiO3, and CaSiO₃ Nano-phosphor

Boris B. Niraula *, Conrad Rizal**

SeedNanoTech and Consulting, Brampton, ON, Canada L6Y 3J6. *Correspondence: <u>boris.niraula@seednanotech.com</u> ** Present address: GEM System Inc, Markham, ON, L3R 5H6. , Canada Email: c.s.rizal@ieee.org

Supplementary Information

The effect of Eu³⁺ ion concentration on X-ray diffraction, XRD, spectra of the phosphor was studied. **Fig. S1** shows XRD patterns of Eu³⁺ doped wollastonite, CaSiO₃ / SiO₃ nano phosphor sintered at 800 °C. Phase analysis indicated that wollastonite type polycrystalline structures dominated these samples. At the same time, tetragonal cristobalite of SiO₂ was also detected in these samples. The wollastonite type crystal orientation is identified with main peaks at 28.8° (-310), 30.0° (112), 36.3° (400) and 39.11° (-240), and these correspond to the triclinic structure. It means that these samples consist of triclinic type unit cell. The tetragonal cristobalite structure due to SiO₂ is identified with main peaks at 22.0° (101), 28.5° (111), 31.5° (102) and 36.2° (200).



Figure S1. XRD spectrum (Intensity vs. $2\theta^{\circ}$) of Eu³⁺ doped CaSiO₃ / SiO₃ nanophosphor powder and its crystallinity. Samples were prepared using a R₀ value of 0.30 and were sintered at 800 °C.

The X-ray diffraction (XRD) profiles in Fig. S2 shows that the intensity of the XRD peak increased monotonously with intensity ratios of (100) and (101), and (002) and (101) peaks with variation in Eu concentration. The ratio of the peak intensities of (100) and (101) progressively increases from un-doped to 5% of Eu doping. Past 2% of doping, it showed a rather small increase, suggesting the dopant concentration is nearing saturation. Likewise, the ratio of the intensity of (002) and (101) peaks showed a similar trend. The only difference is being that past 3% of Eu, a concentration quenching effect is observed. The variation in the latter case is though rather small, while the rate of increase with dopant concentration is higher for the former one. As can be seen, the (100) peak is progressively emerging with increasing Eu. A tendency of enhancing the polycrystalline nature of SiO₂ films appeared with increasing Eu concentration. Finally, with 5% of Eu doping, the intensities of (100), (002) and (101) peaks are almost the same, and it is a quite interesting point to note. The broadening of peaks with doping concentration seems to be due to the substitution of Si⁴⁺ ions by Eu ion with comparatively higher ionic radius.



Figure S2. Effect of Eu³⁺ ion concentration on XRD spectrum (Intensity vs. 20°) of Eu³⁺ doped CaSiO₃ / SiO₂ nano phosphor powder and its crystallinity. Samples were prepared using a R₀ value of 0.30 and sintered at 800 °C.



Figure S3. Effect of Si⁴⁺ concentration on XRD spectra (Intensity vs. $2\theta^{\circ}$) of Eu³⁺ doped CaSiO₃/SiO₂ nano phosphor powder. Samples were prepared in an identical reaction condition using a R₀ value of 0.30 and sintered at 800 °C.



Fig. S4 The energy level of Eu³⁺ doped Eu³⁺ doped CaSiO₃/SiO₂ showing luminescence process and transition states. Adopted from [1].

H. Nagabhushana, B. M. Nagabhushana, M. M. Kumar, K. V. R. Murthy, C. Shivakumara, and R. P. S. Chakradhar, "Synthesis, characterization and photoluminescence properties of CaSiO 3: Eu 3 red phosphor," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 78, no. 1, pp. 64-69, 2011.