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Structure - luminescence relations in Eu-doped thiosilicates

Abstract

Eu^{2+} is considered the doping element of choice in colour conversion phosphors for pcLED (phosphor converted LED) applications. This is because its 5d–4f transition is highly sensitive to the surrounding host, yielding the interesting possibility to tune the emission wavelength by changing the host material. This characteristic can also be used the other way around: the emission spectrum can be used as a probe for structural investigation.

The relationship between the structural and luminescent properties of the europium-doped thiosilicates Ca_2SiS_4 , Sr_2SiS_4 and a series of intermediate compositions of $\text{Ca}_{2x}\text{Sr}_{2-2x}\text{SiS}_4$ ($x = 0, 0.1, \dots, 1$) was studied. Ca_2SiS_4 forms an orthorhombic lattice (space group Pnma, 62) with two non-equivalent lattice sites for Ca^{2+} , which leads to two distinct emission peaks upon doping with Eu^{2+} . Sr_2SiS_4 forms a monoclinic lattice (space group $\text{P}2_1/\text{m}$, 11). In a similar way, europium can be incorporated on two possible Sr^{2+} -sites, leading again to two distinct emission peaks.

Due to the different crystallographic structures, Sr_2SiS_4 and Ca_2SiS_4 are not fully miscible. Single phase powder is obtained for the range from Sr_2SiS_4 to $\text{Ca}_{0.8}\text{Sr}_{1.2}\text{SiS}_4$ and from $\text{Ca}_{1.8}\text{Sr}_{0.2}\text{SiS}_4$ to Ca_2SiS_4 . For the intermediate compositions, phase separation occurs and the luminescence is characterized by four

(partially overlapping) emission peaks, which could be resolved by photoluminescence and cathodoluminescence measurements at low temperature. Upon substitution of Sr^{2+} by Ca^{2+} in Sr_2SiS_4 , the lattice constants reduce, albeit in an anisotropical way. As a consequence, the stronger crystal field causes the emission of europium to shift towards longer wavelengths.

For all compositions, the relation between the structure (as determined using powder XRD and Rietveld refinement) and optical properties was investigated. It was found that Eu-emission can be used as a very sensitive probe of structural changes in the thiosilicates.

Other europium-doped thiosilicate systems (Mg_2SiS_4 , $(\text{Ca},\text{Mg})_2\text{SiS}_4$) and europium doped thiogermanates are under investigation, in order to expand the understanding of the relationship between structure and luminescence in this class of materials.