CRYSTAL STRUCTURE OF Bi/Mn CO-DOPED STRONTIUM ALUMINATE PHOSPHORS

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Strontium aluminate-based compounds have gained much attention due to their outstanding optical properties, high chemical and thermal stability, and wide possibilities for obtaining both bulk and nanostructured highly effective optical phosphors. Recently, research on the activation of aluminates by bismuth and manganese ions has intensified. The luminescence of Bi^{3+} and Mn^{4+} ions in various crystal environments can cover almost the entire visible range, which is important for white LEDs and optoelectronic devices. Of special interest is the sensitization of Mn^{4+} luminescence by Bi^{3+} ions, where the energy transfer efficiency strongly depends on the phase composition and the distribution of activators between the crystalline phases. However, X-ray methods cannot reliably determine the positions of oxygen atoms nor distinguish between neighbouring cations (Sr, Bi, Mn).

In the present work, a set of 16 powder samples of strontium aluminates with systematic variation of dopants (pure matrix, Bi, Mn, and Bi/Mn) and annealing temperatures (1200, 1300, 1400, 1500 °C) was synthesised. The samples were characterised by X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM). It was found that all samples contain a mixture of monoclinic $SrAl_2O_4$ (space group $P2_1$) and cubic $Sr_3Al_2O_6$ (space group Pa-3) phases, with the phase ratio depending strongly on the annealing temperature. The average grain size of both phases is in the nanometre range, as confirmed by SEM and X-ray line broadening analysis. Raman spectroscopy confirmed the incorporation of Bi^{3+} and Mn^{4+} ions into both phases through shifts of the characteristic vibration modes.

Subsequently, a detailed neutron diffraction study was performed at room temperature and ambient pressure using the DN-6 diffractometer at the IBR-2 reactor (Dubna, Russia). Rietveld refinement of the neutron data allowed us to determine the phase fractions, unit cell parameters, atomic coordinates, and site occupancies for both phases. The results show that the cubic phase fraction increases with annealing temperature, while the incorporation of Bi and Mn leads to measurable changes in the Sr–O and Al–O bond lengths. In the co-doped samples, the distribution of Mn is significantly affected by the presence of Bi, providing a structural basis for the Bi→Mn energy transfer mechanism. Luminescence measurements confirm the sensitization of Mn^{4+} emission by Bi^{3+} ions, with the energy transfer efficiency varying systematically with synthesis temperature.

Thus, the combination of XRD, Raman, SEM, and neutron diffraction establishes a direct correlation between the crystal structure and the sensitization efficiency in Bi/Mn co-doped strontium aluminates. These findings enable rational design of high-performance phosphors for white light-emitting diodes and other optoelectronic applications.