Realization of White Light Emission as a Manifestation of Dy\(^{3+}\) to Eu\(^{3+}\) Energy Transfer in Single Component MgAl\(_2\)O\(_4\): Dy\(^{3+}\), Eu\(^{3+}\) Nanophosphor: A Promising Candidate For Solid State Lighting & Self referencing Optical Thermometry Applications

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**Method of Rietveld analysis:**

The Rietveld method of powder structure refinement\(^{1-2}\) is one of the best known methods to ascertain different (micro/nano) structure parameters of single/multi-phase materials. Adoption of this method becomes incumbent for quantitative phase analysis of a multiphase material where reflections from the constituent phases are severely overlapped. The experimental XRD pattern is simulated using analytical functions that depend on different structural and microstructure parameters of each individual phase.\(^3\) The calculated intensities \((y_{ic})\) are determined from the following equation:\(^3\)

\[ Y_{ic} = S \sum_k L_k |F_k|^2 \Phi(2\theta_i - 2\theta_k) P_k A + y_{bi} \]  

(1)

where \(S\) is the scale factor, \(k\) represents the Miller indices \((h,k,l)\) for a Bragg reflection, \(L_k\) represents the Lorentz polarization and multiplicity factors, \(\Phi\) is the reflection profile function, \(P_k\) is the preferred orientation function, \(A\) is absorption function, \(F_k\) is the structure factor for the \(k\)th Bragg reflection and \(y_{bi}\) is the background intensity of the \(i\)th step. Marquardt least-square refinement procedure is used to monitor the difference between the observed and the calculated pattern with the help of the reliability index parameters, \(R_{wp} = \left[ \frac{\sum_i w_i (Y_{io} - Y_{ic})^2}{\sum_i w_i Y_{io}^2} \right]^{1/2} \) (weighted residual error), and \(R_{exp} = \left[ \frac{(N-P)}{\sum_i w_i Y_{io}^2} \right]^{1/2} \) (expected error). Where \(w_i\) is the statistical weight, \(Y_{io}\) and \(Y_{ic}\) are the observed and calculated X-ray diffraction intensity, \(N\) is the weight and number of experimental observations and \(P\) is the number of fitting parameters. Goodness of Fit (GoF)\(^4-5\), which is the ratio of \(R_{wp}\) and \(R_{exp}\), indicates the refinement quality. The peak shape is assumed to be to be a pseudo-Voigt (pV) function with asymmetry to take into account the individual broadening caused by particle size and strain respectively.\(^6-7\) In the present study, Rietveld software MAUD (Materials Analysis Using Diffraction)\(^8\) version 2.79 is utilized for simultaneous
refinement of different structural and microstructure parameters of MgAl$_2$O$_4$:Eu$^{3+}$, Dy$^{3+}$ nanostructures.

**Figure S1:** FTIR of synthesize samples.

**Figure S2:** XPS survey scan of Eu$^{3+}$, Dy$^{3+}$ co-doped MgAl$_2$O$_4$ nanophosphor
Figure S3: (a) PL excitation (left side, monitored at 575 nm) and emission spectra (right side, excited by 351 nm) of MGA: 2% Dy\textsuperscript{3+} nanophosphors (b) PL excitation (left side, monitored at 616 nm) and emission spectra (right side, excited by 394 nm) of MGA: 2% Eu\textsuperscript{3+} nanophosphors.

Figure S4: PL spectra of MGA: 2% Dy\textsuperscript{3+}, 0.2% Eu\textsuperscript{3+} and reference sample (Benflect recorded in an integrating sphere attached with PL spectrometer for quantum yield measurement.)
References:


