

Mathematical modeling of emission bands of fluorite and its implications Maisnam Bidyasagar¹, Lisham Paris Chanu² and R. K. Gartia²

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Abstract

In this paper, we have demonstrated the parameterization of photoluminescence (PL) spectra of an Indian fluorite using Gaussian function as the mathematical profile. The deconvolution reveals the dominant broad violet emission at 2.87eV/432nm with full-width at half maximum (FWHM) 0.245eV for 340nm excitation. For excitation with 270nm in addition to the broad violet emission, sharp lines are also observed with FWHM ~0.035±0.004 eV. The motivation for the work is that spectral bands and lines must be parameterized in terms of their position (ϵ_{max}), FWHM (W) and intensity maximum (I_{max}) and not only the position. As for green Indian fluorite the emission is spread over the wide range of 400- 550nm with a prominent violet band. It is correlated with Eu²⁺. With Eu²⁺ as the activator, green fluorite is expected to be a natural phosphor emitting in a zone sensitive to all common photomultiplier tubes offering its candidature as a natural TLD. However, correlation of all the deconvoluted bands and lines with specific recombination center requires further studies, since fluorites in general contain practically all rare-earths, their concentration being dependent on the source materials.

.Keywords: Photoluminescence (PL,) Indian Fluorite (Green), emission band and line.

1 INTRODUCTION

Mathematical models are used very commonly in all branches of natural sciences as well as engineering sciences. Models are needed to check theoretical concepts by comparing them with experimental results. The model may be simple or complex depending upon the necessity as well as complexity of the phenomenon. In the case of photoluminescence (PL) of materials, spectral line/band shapes are generally deconvoluted using Lorentzian, Gaussian or Voigt functions that parameterised the profile of the line/band in terms of their position, Full width at half maximum (FWHM) and the maximum intensity. In this communication we deconvolute the PL spectra of Indian fluorite (green) using Gaussian function essentially to distinguish the emission in terms of bands and lines, identify the impurities in the mineral that the emission matches with standard literature data and infer some potential areas to show that PL, a simple technique can be used to authenticate fluorescent minerals as phosphors without resorting to expensive techniques for check-up. Practically, naturally occurring fluorites of different origin have rare earths as impurities [1-6]. Fluorites are known to have numerous divalent and trivalent rare earth impurities which give rise to emission spectra of both broad band as well as narrow line characteristics. Rare earth recombination centres in fluorites which give rise to luminescence emission can be classified as bands and lines based on their FWHM. Eu²⁺ and Ce³⁺ ions are known to have broad emission, whereas trivalent rare earths viz. Eu^{3+,} Tb³⁺, Tm³⁺, Dy³⁺, Sm³⁺, Ho³⁺, Er³⁺ etc. are known for line emission [7-8].

2 EXPERIMENTAL DETAILS

The fluorite mineral used in this work is Indian green fluorite. Using X-ray diifraction and Energy Dispersive Xray analytical technique, the sample was confirmed to be pure CaF_2 without any other associated minerals. The emission spectra of the fluorite used is recorded with Photoluminescence Spectrophotometer, Perkin Elmer (precisely LS-55 Fluorescence spectrometer Edinburg Instrument UK). PL emission spectra recorded with different excitation wavelength are deconvoluted with Gaussian function using commercial PeakFit software.

3 RESULTS AND DISCUSSION

The emission spectra of the sample spread over the range 400 to 550nm and extended to~ 450nm to 700nm for excitation with higher energy. The PL spectra of the sample consist of dominant violet emission band at 2.87 eV (432 nm) with FWHM 0.245 eV for excitation wavelength with $\lambda = 340$ nm. This broad emission can be correlated with Eu²⁺ ion [3-4]. But many sharp lines around 2.33eV (532 nm), 2.51eV (494 nm), 2.54eV(487 nm) and 2.80eV(444 nm) with FWHM ~0.035\pm0.004 eV are superimposed for



excitation wit $\lambda = 270$ nm and $\lambda = 263$ nm. Fig.1 shows the normalised emission spectra of the sample excited with light of different wavelengths. The prominent broad violet emission can be correlated with Eu²⁺ ion, whereas the sharp lines can be assigned to other trivalent rare earths.

Fig.2 shows the difference of the emission spectra for excitation with wavelength 270 and 340nm. The deconvoluted signals of the curved is shown in Fig.3 which is fitted with sixteen band and line emission.

The deconvoluted signals is parameterised in terms of intensity, FWHM(eV), peak position(eV) where its best fitted components are shown in Table 1. From the FWHM values, the emission signals can be classified as bands and



Fig.1: PL emission spectra of Indian green fluorite.

Table1: Parameters of emission bands/lines in addition to the dominant Eu²⁺ emission.

. 4 **CONCLUSION:** Fluorite in general can be used as natural TLDs, since they have bountiful emission centers emitting in ranges ideal to match sensitivity of photo-multiplier tubes, coupled with the fact that they do exhibit stable TL peaks. However they need to be characterised for the trace rare earth constituents to get precise information.

sharp lines, whose emission centres can be correlated with standard data to identify the rare earth recombination centres [9]. But assigning a particular line emission to a particular electronic transition of a trivalent rare earth require details about the individual trace rarre erath impurities and and precise TL study.



Fig.2: Residue for emission with excitation wavelength 270nm and 340 nm.



Fig.4: Gaussian deconvoluted emission spectra of the residue curve of fig.3.

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Table-1

Peak	Amp.	Center (eV)	λem(nm)	FWHM
Ι	0.28	1.76	705	-
II	0.98	1.90	654	0.104
III	1.32	2.00	619	0.101
IV	2.26	2.07	599	0.082
V	3.44	2.16	573	0.092
VI	2.66	2.23	557	0.063
VII	5.61	2.28	544	0.063
VIII	5.09	2.33	532	0.039
IX	11.97	2.39	519	0.142
X	11.00	2.48	500	0.086
XI	4.71	2.51	494	0.035
XII	13.52	2.54	487	0.039
XIII	22.13	2.58	480	0.128
XIV	9.60	2.69	462	0.083
XV	6.82	2.76	450	0.064
XVI	1.93	2.80	444	0.031