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STRUCTURAL AND MECHANICAL PROPERTIES ON Tb^{3+} DOPED KBr SINGLE CRYSTALS

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Abstract:- *Tb^{3+} doped KBr single crystals is grown by Bridgeman Stockbarger technique. The grown crystal was subjected to powder X-ray Diffraction (PXRD), Fourier Transform Infrared analysis (FTIR) and Vicker's microhardness (H_v). The average crystallite size was calculated using well known Debye Scherrer's formula and found in the range of 8.5μm. The presence of various functional groups has been identified from FTIR studies with their vibrating frequencies. The mechanical property was studied by vicker's microhardness indenter. Vicker's hardness value (H_v) are calculated for selected applied load and it is found to be increasing with increasing applied load. The Mayer's index number(n) is calculated to be 0.3, the crystal system belongs to hard material category. The Elastic stiffness constant (C_{11}) value is $5989X10^{11}$MPa which is calculated using Wooster's empirical relation.*

Keywords: *XRD, FTIR, Vicker's microhardness*

1. Introduction

In recent years, the new lighting and display technology such as LEDs and FEDs have been proposed in industry, which result in the luminescence associated with Tb^{3+} content in different host lattices has found applications[1-6]. Tb^{3+} ion has the $4f^8$ electron configuration undergoes 4f→5d transition and this electron excited state is $4f^7 5d^1$[7]. The last few decades a lot of luminescence studies have been reported on alkali halides doped with rare earth ions[8,9]. The band gap of alkali halide also has a wide range, varying from 7.34Å for RbI to 4.03Å for LiF[10,11]. In the present work Tb^{3+} doped KBr crystals has been grown by Bridgeman Stockbarger method and the grown crystals was subjected to structural, vibrational and mechanical properties.

2. Experimental Detail

Single crystals of Tb^{3+} doped KBr (99.99% purity) were grown using Bridgeman Stockbarger technique. Tb^{3+} was added in the form of Terbium fluoride (Aldrich; 99.99% purity). The crystals were grown in three different concentrations with impurities of 1%, 3% and 5% by weight. The studies were performed on crystals of all three concentrations. The results obtained were similar but changed in intensity in accordance with the concentration of the impurity. Hence, as a representative, the results obtain pertaining to the 3% concentration are presented and discussed. X-ray diffraction spectrum of the prepared sample by using (Rigaku) X-ray diffractometer (CuK_α, λ=1.54060Å) and the variation of 2θ is from 20° to 90°. FTIR spectra were measured using a Perkin Elmer spectrometer within the range of 400-4000 Cm^{-1}. The mechanical property of the grown crystals has been studied using a Vicker's hardness tester.

3. Powder X-ray Diffraction Pattern

In order to determine the crystal structure and phase purity of the crystals, x-ray diffraction analysis was carried out. **Fig.1** shows Powder X-Ray Diffraction pattern of the Tb^{3+} doped KBr crystals. XRD data of Tb^{3+} doped KBr crystals were collected from a X-ray diffractometer CuKα radiation. From the PXRD pattern analysis it was found that the prominent phase formed was KBr, intensity and hkl values presented in the **table.I**. The KBr phase belongs to the space group Fm3m having a hexagonal crystallite structure. The miller indices (hkl) compared with the JCPDS Card No:04-0531 of pure KBr The lattice parameters were found to be α=β=γ=90°, a=b=6.6(Å), c=9.3(Å). The cell volume is $485(Å)^3$. The intense peak observed at 2θ values of 23.4° to 89.4°. XRD spectrum of KBr:Tb^{3+} crystals exhibits intense peak located at 2θ=27°. The peaks corresponding to the hkl planes is [2,0,0]. The crystallite size of KBr:Tb^{3+} crystals is estimated using Scherer's formula[12], where, "D" is crystallite size, "k" is the Scherer's constant

(0.94), "λ" is the wavelength of X-ray (1.54060 Å), "β" is the full width half maxima, θ- is the Bragg angle. The crystallite value was found to be 8.5µm.

4. Fourier Transform Infrared

The FTIR spectra are useful to identify the functional groups present in the samples and these spectra of Tb^{3+}doped KBr crystals were recorded using Perkin Elmer FTIR spectrometer in the range 400-4000cm^{-1} as shown in **Fig.2**. It exhibits a broad absorption band in the region 3383cm^{-1} assigned to O-H stretching vibration.

5. Vicker's Microhardness

Microhardness analysis was carried out for the grown crystal using vicker's microhardness tester fitted with a diamond indenter. Hardness is measure of resistance of the material to plastic deformation. The hardness of the mechanical plays a significant role in device fabrication. The hardness of the crystal carriers information about the mechanical strength and molecular binding of the material. The vicker's microhardness tester and the loads of different magnitude were applied over a fixed interval of time and the hardness was calculated using the relation, $H_v=1.8544\ P/d^2\ (kg/mm^2)$**[13]**, where , P is the applied load (Kg) and d is the diagonal length of the indentation impression (mm). The variation of H_v increases with increasing the applied load P is shown in **Fig.3**. A plot of logP versus logd for the grown crystal is shown in **Fig.4.** The plot yields a straight line graph, and its slope gives the work hardening co-efficient(n). According to Onitch**[14]** and Hanmann**[15]**, n lies less than 1.6 for hard materials and is greater than 1.6 for soft material. The "n" value observed in the present studies is 0.3 suggesting that the grown $KBr:Tb^{3+}$ crystals is a relatively hard material category.

The Elastic stiffness constant is a measure of the resistance of the material to deformation. The Elastic stiffness constant(C_{11}) for different loads are calculated using Wooster's Empirical formula $C_{11}=H_v^{7/4}$ **[16]** and is shown in **Fig.5.** The stiffness constant gives an idea about the tightness of bonding with the neighbouring atoms. In the case of $KBr:Tb^{3+}$ crystals, the stiffness constant is found to increase with the applied load. Elastic stiffness constant with different loads as shown in **table.II**.

Conclusion

Tb^{3+} doped KBr single crystals have been grown successfully from Bridgeman Stockbarger technique. The functional groups were identified by FTIR spectroscopic analysis. The microhardness of the crystals was tested by Vicker's hardness and it shows that the crystal hardness increased for various loads. Hardness test revealed that the grown crystal $KBr:Tb^{3+}$ is belonging to hard material category. PXRD analysis that grown material is crystallized in hexagonal system with in a space group Fm3m.

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FIGURE No.1

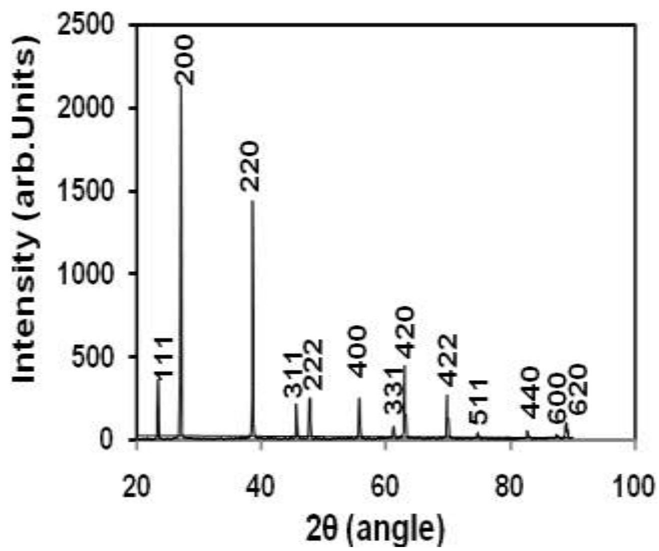

Fig.1 XRD pattern of Tb^{3+} doped KBr crystals

FIGURE No.2

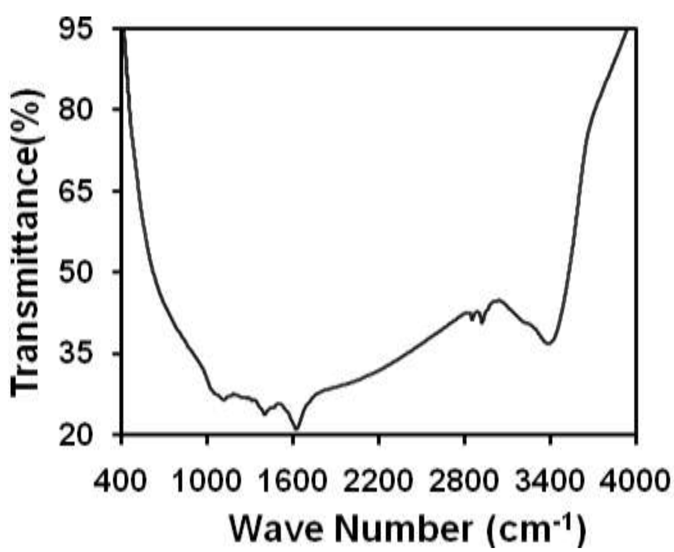

Fig.2 FTIR spectrum for Tb^{3+} doped KBr crystals

FIGURE No.3

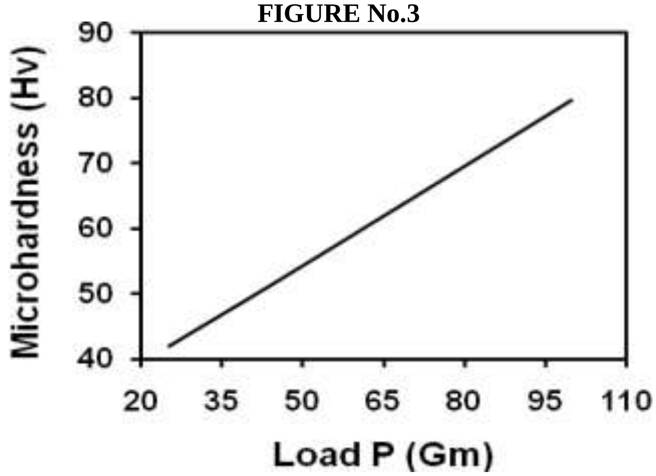

Fig.3 The Plot of load P Versus Microhardness for Tb^{3+} doped KBr crystals

FIGURE No.4

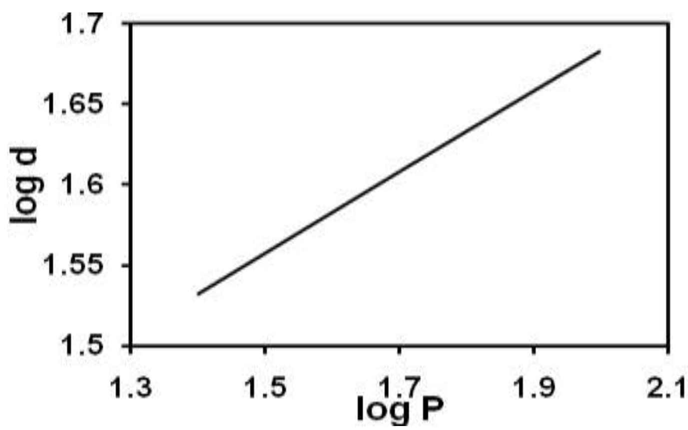

Fig.4 The Plot of log p Versus log d for Tb^{3+} doped KBr crystals

FIGURE No.5

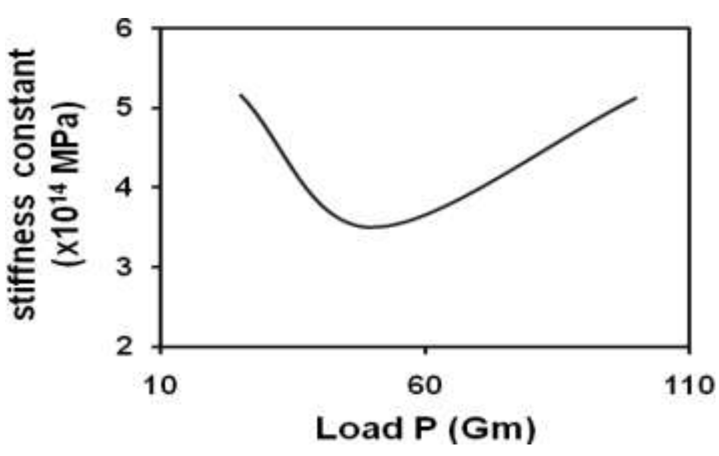

Fig.5 plot of load p versus elastic stiffness constant of Tb^{3+} doped KBr single crystals

TABLE No.I

Table.I. 2θ , intensity and hkl values of Tb^{3+} doped KBr crystals.

S.No	2θ (degree)	Intensity (arb.U)	hkl values
1.	23.4	358	111
2.	27	2128	200
3.	38.6	1436	220
4.	45.6	223	311
5.	47.8	242	222
6.	55.7	255	400
7.	61.2	82	331
8.	63	449	420
9.	69.8	273	422
10.	74.7	44	511
11.	82.7	60	440
12.	87.4	36	600
13.	88.9	105	620

TABLE No.II

Table.II Elastic stiffness constant with different loads for Tb^{3+} doped KBr crystals.

Load P(g)	C_{11} (10^{14}MPa)
25	5.1715×10^{10}
50	3.5021×10^{11}
100	5.1292×10^{12}