INFRARED AND RAMAN SPECTROSCOPY STUDY OF $Y_3Al_5O_{12}$ NANOCERAMICS DOPED 50% Ho+3

I.Ianez[1], B.Rekik[1], M.Derbal[1].

[1]LASICOM Laboratory, Faculty of Sciences, Saad Dahleb Blida 1 University.

ABSTRACT

The cubic garnet is one of the most important categories of materials. Essentially it dedicated to the field of Optics: Yttrium Aluminum Garnet (YAG) representing a host of good choice matrix. In this research work, we made the synthesis by reaction in the solid state; to get high powder (YAG) ceramics quality doped 50% with trivalent holmium ions. Deep phonon vibrational studies on optical properties by IR spectroscopy and Raman of the compound $Y_3Al_5O_{12}$ (YAG) doped 50% Ho^{+3} presented by the spectra IR and Raman sets or the characteristic IR absorption bands of bonds M - O (M = Y, Al) and active modes of internal vibration associated with the different frequencies of the material YAG: 50% Ho^{+3} are confirmed through the spectra of IR and Raman of the YAG respectively **[1.2].**

Keywords: cubic garnet; trivalent holmium; phonon vibrational studies; FT-IR; Raman.

Author Correspondence, e-mail: imanelanez@mail.com

1. INTRODUCTION

$A_3Al_5O_{12}$ Cubic Garnet materials have become the great choice for the development of new materials that are very favorable to optical applications, especially laser visualization, these host matrices have the desired characteristics: (physico-chemical, mechanical, optical, thermal ...) Yttrium Garnet Aluminum (YAG) is the famous known example because of its hardness and good conductivity, etc… **.** The structure of doped or not doped $Y_3Al_5O_{12}$ (YAG) material

belongs to space group Ia3d and crystallizes in a cubic system with a cell parameter of 12 Å, the elemental cubic cell contains eight form patterns (160 atoms). In this cubic structure, all the oxygen is identical to the number of 96 atoms per unit cell. Yttrium occupies the dodecahedral positions (24 atoms per unit cell) while the aluminum ions are found in two different octahedral sites (16 atoms per unit cell) and tetrahedral (24 atoms per unit cell) **[3].**

In order to broaden the scope and spectroscopic properties of $Y_3Al_5O_{12}$, it is generally doped with trivalent rare earth ions. The new one in this study is the doping of this cubic garnet matrix $Y_3Al_5O_{12}$ by 50% of the trivalent holmium ions, so there is a preferential site for the Ho^{3+} doping ion, it is the dodecahedral sites in substitution of the Y^{3+} ions, to have after a scintillation material instead of having a laser effect.

In this paper, we will expose, and discuss the optical spectra found by infrared and Raman spectroscopy of YAG ceramics doped 50% Ho^{+3} nanocrystals manufactured by the solid-state reaction method.

2. Experimental processes

The Powder $Y_3Al_5O_{12}$ ceramics doped 50% with the holmium ions are elaborated (YAG: 50% Ho^{+3}) by the solid state reaction method. High purity compounds were used for the synthesis: Yttrium oxide (99.99%), Aluminum oxide (99.99%), with the doping oxide it is the Holmium one (99.99%) are well prepared and mixed thoroughly in an agate mortar, cold pressed at 4000 kg cm^{-2} into rectangular pellet of 30 mm in length and 0.3 mm^2 in section. and are maintained at a synthesis temperature of 1450 ° C during a long time, about dozens of hours in the following reaction The samples were synthesized by the solid state reaction accordingly to the following chemical equation:

$$5Al_2O_3 + 1.5(Ho_2O_3 + Y_2O_3) \rightarrow 2(Y,Ho)_{1.5}Al_5O_{12}$$

After the preparation and elaboration of YAG, powders ceramics, doped with 50% Ho^{+3}, the prepared pellets shown in fig .1 were ground once more for further measurements. we launched the studies of characterizations by the X-ray patterns which they were obtained with a Bragg-Brentano Bruker D8 Advance diffractometer working with the Cu Ka radiation, thanks to a backward monochromator, then we also detailed the optic studies of characterization by the Infrared spectroscopy using a JASCO-4100 FTIR Fourier Transform Spectrometer as KBr pellets in the 4000–500 cm^{-1} region, and Raman Spectroscopy using a Horiba JobinYvonAramis where it was recorded at room temperature using a micro-

spectrometer Horiba Jobin-Yvon ARAMIS for excitation by 473 nm and 633 nm lines with a He Cd UV laser and He–Ne laser respectively.

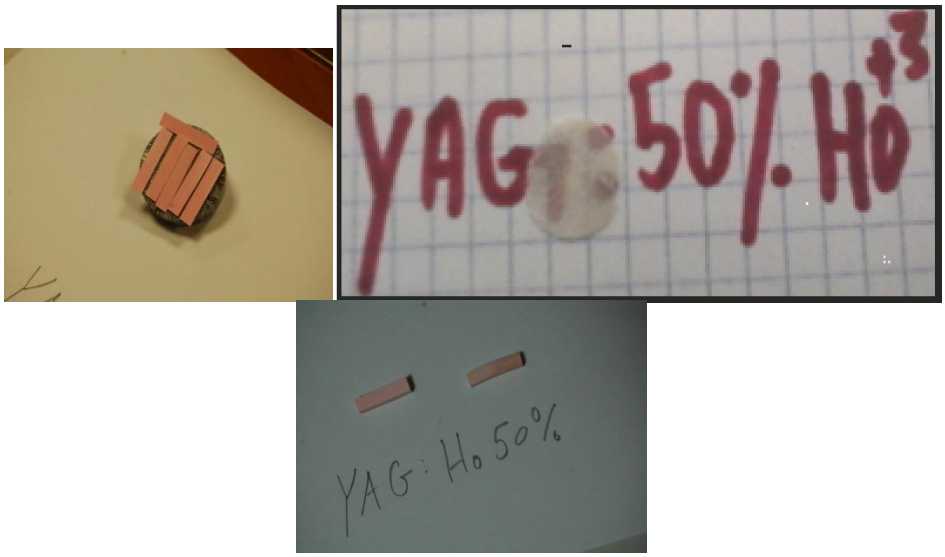

Figure 1: Photos of powder samples of YAG doped 50% Ho^{+3}

2. Results and Discussion

XRD experimental patterns were used to calculate density, lattice parameters and crystallite size in the nanoceramis .The structural study by X-ray diffraction was carried out, **Fig. 2** shows the X-ray diffraction pattern on YAG doped 50% Ho^{+3} synthesized.

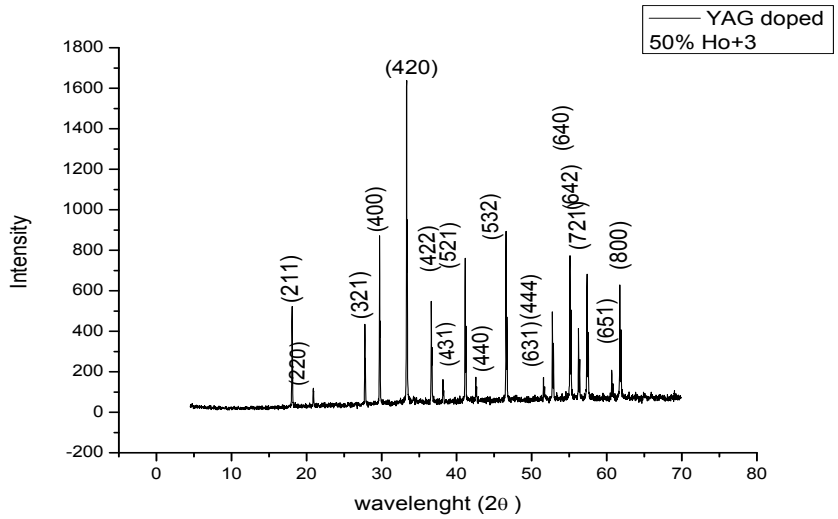

Figure 2: DRX diffractogram of 50% Holmium-doped $Y_3Al_5O_{12}$.

From the identification of the X-ray diffractogram peaks of Ho^{+3} doped YAG and the Bragg condition: ($2d_{hkl} \sin\Theta = n\lambda$), we confirmed that the pure garnet phase which this material crystallizes in a cubic structure with a cell parameter, (a = 12 A°).

For the YAG which crystallized in cubic systems and O_h space group, the group theory predicts **3A1g + 5A2g +8Eg + 14T1g + 14T2g + 5A1u + 5A2u + 10Eu + 18T1u + 16T2u** Brillouin zone center modes where it predicts 25 Raman active modes only **the (3 A1g+8 Eg,+14T2g)** and 17 IR active modes of **T1u** symmetry. **[4],** for that reason there have been phonon vibrational studies IR and Raman to better understand the structures (bonds types, vibrational modes associated in a different frequencies ,…) of the YAG doped 50% Ho^{+3}.

The FTIR spectrum of YAG doped 50% Ho^{+3} **(Fig. 3),** deviated by two intervals, the first interval is started from 500-1000 cm^{-1}, we find here the appearance of the differents modes of vibrations (stretching, bending) associated with the different frequencies **515, 569,696, 513, 724, and 789 cm^{-1}**, also the different types of bands M-O (M = Y, Al), of the host matrix $Y_3Al_5O_{12}$ elements , for the second range, it is started from 1000 cm^{-1} to the end of the spectrum , here we obtained to others types of vibrations, these are external vibrations like H-O, C-H ect ...

The Raman spectra **(Fig. 4)** of YAG doped with 50% Ho^{+3} excited with 633 and 573 nm represent the Raman bands characteristic associated with the differents frequencies similar to those of the YAG published in the literature , Raman spectra of YAG nanocrystals powder and ceramics are similar to the spectrum of a single crystal also. These well resolved and intense bands **372, 462, 596, 647, 721, and 835 cm^{-1}**are marked on (YAG: 50% Ho^{+3}) corresponding stretching, bending modes with others external vibrations.

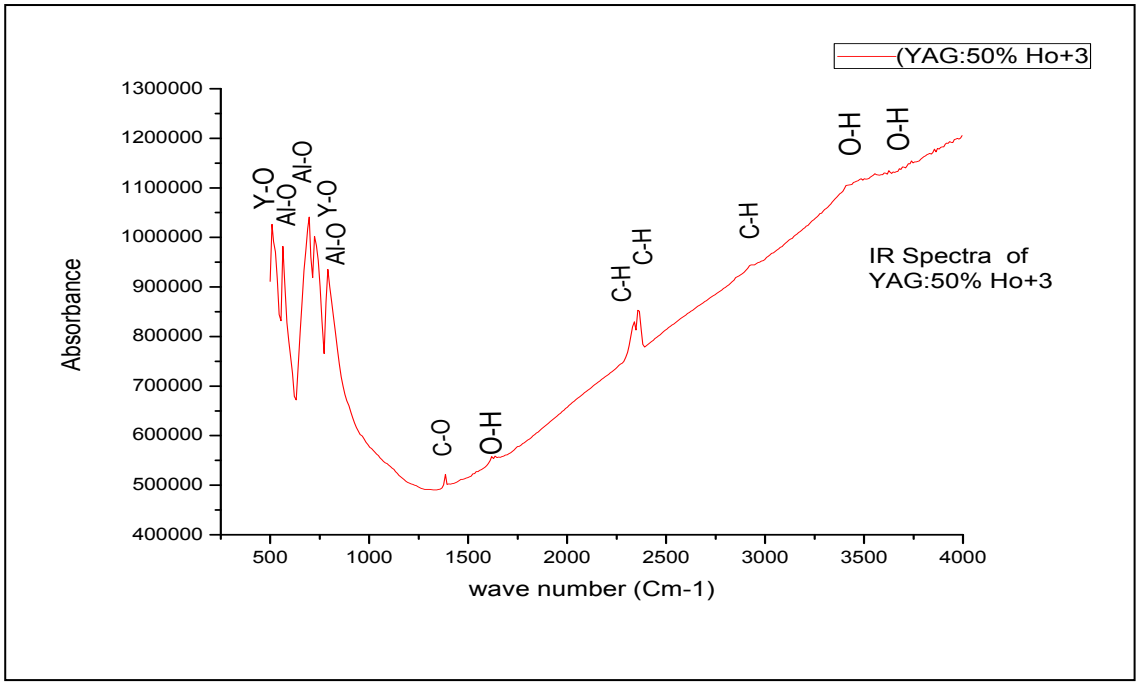

Figure 3: FTIR spectrum of YAG: 50% Ho $^{+3}$

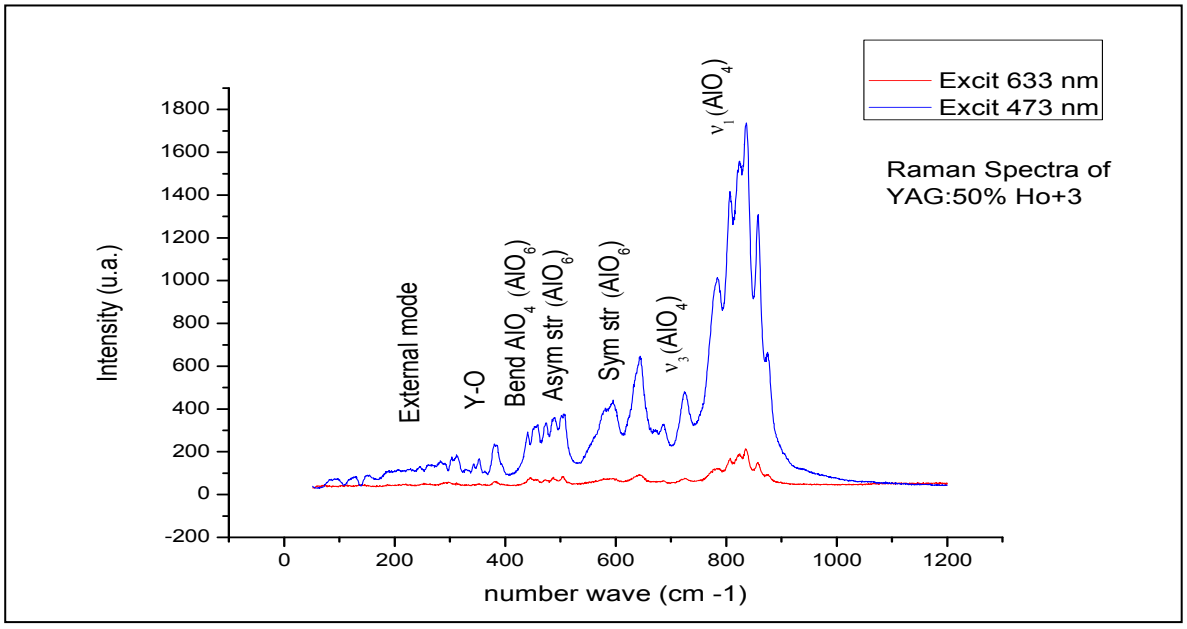

Figure 4: Raman spectra of YAG: 50% Ho $^{+3}$

The **table 1** in bellow summarizes all the results represented by all the frequencies and the identification of the vibration modes obtained.

Table 1 Vibrational Assignment of at 50% H^{3+} doped YAG powder

YAG:50 % Ho+3	Positions of bands (cm-1)	Vibration modes [1,2,5,6]	YAG:50 % Ho+3	Positions of bands (cm-1)	Vibration modes [1,2]
IR Bands	515.785	Y-O	Raman Bands	835.820	υ_1AlO4
	569.098	Asy.stretching AlO6		721.890	υ_3AlO4
	696.111	Sym.stretching AlO6		647.263	Sy.Stret (AlO6)
	738.448	Stretching Y-O		596.019	Asy.str (AlO6)
	790.978	AlO4		462.688	Bend AlO4 (AlO6)
IR Bands	1384.486	C-O	Raman Bands	372.636	Y-O
	1649.487 [3000-3600]	O-H		[82.089-309.950]	External mode
	2370.008 ;2900	C-H			

4. CONCLUSION

In this work, we have studied and characterized by IR and Raman spectroscopy the optical properties of $Y_3Al_5O_{12}$ powder doped 50% with trivalent holmium ions by the solid-state reaction method. The results by structural analysis (XRD) carried out on the powders $Y_3Al_5O_{12}$: 50% Ho^{+3} confirmed the existence of the pure garnet phase. So the analysis carried out by IR absorption spectroscopy and Raman scattering on this new material ceramic (YAG: 50% Ho^{+3}) demonstrated the presence of the absorption bands at well-determined frequencies by several comparing with published frequencies to identified and proved the crystal structure.

5. REFERENCES

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