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STRUCTURE AND OPTICAL PROPERTIES OF $GdYMoO_6$ NANOCERAMIC

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Gadolinium molybdate has many applications in ferro electricity, laser hosts, phosphors and catalysis. Yttrium molybdate is a promising material in Near Ultra Violet (NUV) excited white LED's. In the present work $GdYMoO_6$ nano particles are synthesized by combustion method followed by a heat treatment at 900^oC. The prepared materials are characterized by X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR) and UV-visible spectroscopy. The X-ray diffraction studies show that $GdYMoO_6$ crystallize in a monoclinic structure with space group I2/a (15). The lattice parameters obtained from the XRD analysis are in good agreement with the reference data. The average crystalline size calculated by Scherer's method is about 39 nm. The IR spectrum shows only the bands corresponding to the metal oxygen bond vibrations such as Gd-O, Mo-O, and Y-O. The UV – visible absorption spectrum indicates that the material has a heavy absorption in the UV region. The direct bandgap calculated from the Tauc's plot analysis 3.45eV.

Keywords: Combustion synthesis, nanoceramic, bandgap.

INTRODUCTION

Nanoceramics can be used for variety of applications due to their electronic and optical properties[1].Combustion synthesis is considered as an effective technique for the synthesis of nanomaterials. Solution combustion process can be used for the preparation of ceramic oxide powders and it is based on the combination of aqueous solution of metal nitrates with a fuel[2].Rare earth doped luminescent materials have applications in various fields, such as optoelectronics, fiber amplifiers, solid-state lasers and phosphors[3]. The rare earth ions were characterized by a partiallyfilled 4f shell,shielded by $5s^2$ and $5p^6$ orbitals. Since rare earth ions have the same electric charge and similar radius, they can be easily replaced by each other in the host, which always leads to efficient phosphors with special optical properties[4].Molybdates have broad and intense charge transfer absorption bands in the near UV wavelength and has excellent thermal and chemical stability[5]. In this paper, we report the structure and optical properties of GdYMoO6 nanoceramic, prepared through an auto-igniting combustion technique.

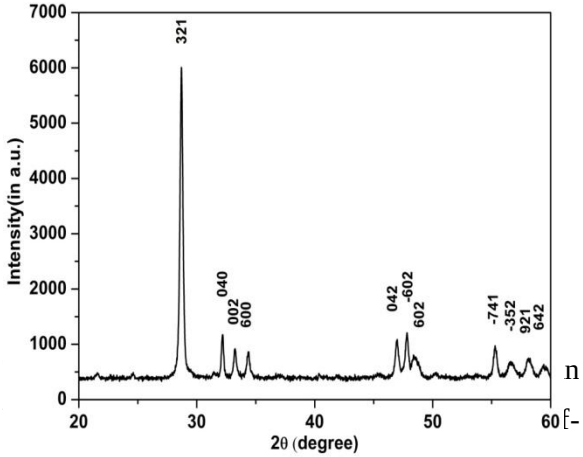
Experimental

The sample is prepared through combustion technique using the corresponding metal nitrate

(oxidizing agent) and suitable fuel (reducing agent).Calculations are based on the principles of propellant chemistry, keeping the fuel-to-oxidant ratio as unity to produce maximum energy[6]. The starting materials areGadolinium oxide (Gd_2O_3, 99.9%), Yttrium oxide (Y_2O_3) and Ammoniumhepta molybdate $(NH_4)_6Mo_7O_{24}.4H_2O$. The rare earth oxides are dissolved in nitric acid and urea (NH_2CONH_2) is added as fuel reagent (reducing agent). Citric acid is used as complexing agent to form the precursor complex[7]. Stoichiometric amounts of oxidizing and reducing agents are dissolved in a minimum volume of deionized water to obtain transparent aqueous solution in a glass beaker, which is subsequently heated using a hot plate at 250^0C in a ventilated fume hood. The solution boils on heating and undergoes dehydration accompanied by foaming. On persistent heating, the foam gets auto ignited, giving a voluminous fluffy powder of $GdYMoO_6$. The powder obtained after auto-ignition is annealed at 900^0C for one hour to obtain pure, nanocrystalline powder. The prepared samples are characterized by using X-ray diffractometer (D8 advance, Bruker, Germany) with CuKα radiation in the range of 20–70 in steps of 0.02. The infrared spectrum of the samples is recorded in the range 400–1000 cm^{-1} on a Fourier Transform Infrared (FTIR) Spectrometer (Spectrum2, Perkin-Elmer, Singapore) using the ATR method. Particle properties of the prepared nanoparticles are imaged using high resolution transmission electron microscopy (Jeol/JEM 2100, USA) operating at 200 KV. The diffuse reflectance spectrum of the sample is recorded in the range 200 to 800 nm using a UV-Vis spectrometer (Lamda 35, PerkinElmer, Singapore) with an integrated sphere accessory (RSA-PE-20, Lab sphere, USA).

Results and discussions

The XRD diffraction pattern of $GdYMoO_6$ powder annealed at 900^oC,shown in fig: 1 is used forthe structural analysis of the sample.All the peaks can be indexed for a monoclinic structure with space group I2/a (15). The lattice constants calculated from the XRD analysis are a=15.66A^0, b=11.12 A^0 and c = 5.71A^o. These values are in good agreement with the reference JCPDS card No. 24-0423



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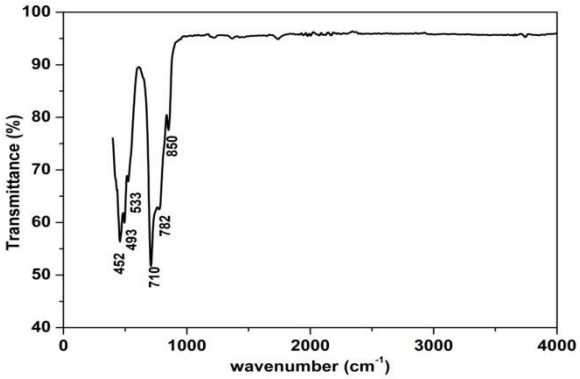
maximum (FWHM) of the diffraction peaks using the Scherrer formula,

$D=K\lambda/\beta \cos\theta$

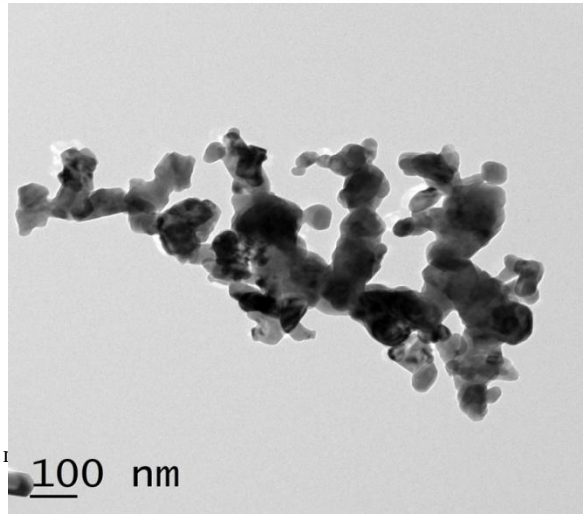
where D is the crystal size, λ is the $CuK\alpha_1$wavelength (1.5406 Å),β is the full width

half maximum of the peak in radian and θ is the corresponding diffraction angle. The average particle size calculated by this method is about 39.10nm.

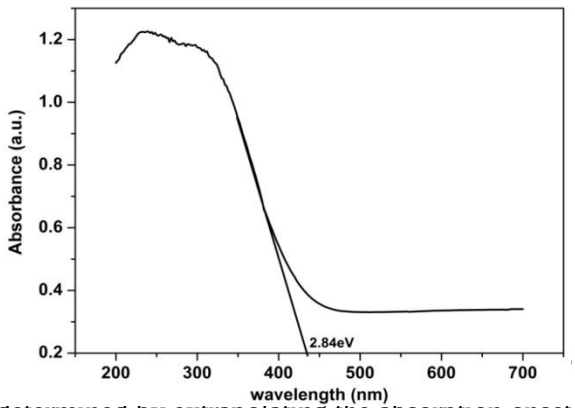
The Fourier Transform infrared (FTIR) spectrum of the sample recorded in the range 400–4000 cm^{-1} with a resolution of 4 $cm^{-1}$is shown in fig: 2. This spectrum shows only the metal oxide vibrations of the prepared compound.The main peak at 710-850 cm^{-1} is ascribed to Mo-O vibrations and weak peak at 533 cm^{-1} is due to Gd-O bond vibrations [3]. Other absorption bands between 620 and 900 cm^{-1} are due to the vibrations of Y-O bond. Also the absorption bands between 430 and 600 cm^{-1} is due to metal Mo-O vibrations [8].



visualization of nanosized $GdYMoO_6$. Fig:3 shows the TEM image of the prepared material and it can be seen that the particles are slightly agglomerated. The average particle size calculated from the image is nearly 45 nm, which is comparable with the XRD results.



The UV–visible absorption spectrum is recorded in the range 200 to 800nm to characterize the optical absorbance of the as-prepared nanoceramic. The measured absorption spectrum of the prepared material is shown in fig: 4. From the figure it is clear that the sample absorbs heavily in the UV region. Also, this material shows an exponential decrease with increase of wavelength.



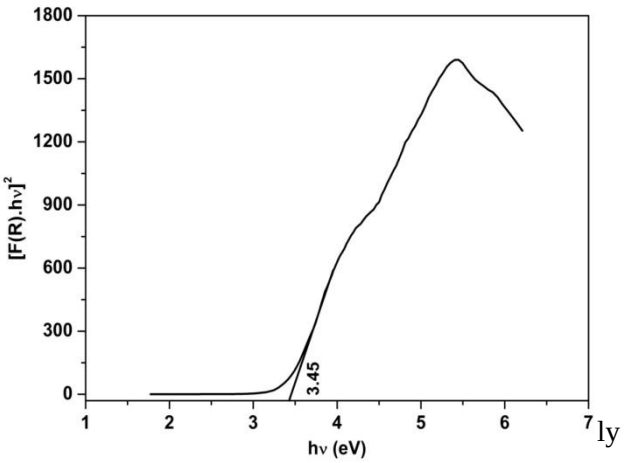
determined by extrapolating the absorption onset in the UV region to the X-axis. The intersecting wavelength is then converted into corresponding energy using the relation E = hc/λ.The

absorption band edge wavelength and corresponding energy value are 438.5nm and 2.84 eV respectively.

The dependence of optical bandgap in the absorption photon energy can be modeled by using Tauc's equation,

$$(\alpha h\nu) = \mathbf{B}\ (h\nu - E_g)^m$$

Where,B is an energy independent constant, α is the absorption coefficient, E_g is the optical band gap energy, h is Planck's constant, ν is the frequency of incident photon and m is an index which depends on the nature of electronic transition responsible for the optical absorption. The value of m is 1/2 and 2 for allowed direct and indirect transitions, respectively. The optical transition for Gd_2MoO_6 nanomaterial is previously reported as direct bandgap[9]. Tauc's plot drawn for the $GdYMoO_6$ is shown in fig:5. Extrapolating the linear part of the plot to X-axis gives the bandgap energy of the material as 3.45eV.



ly prepared by auto-igniting combustion method. The XRD results indicate that GdYMoO6 can be assigned to the monoclinic structure. FTIR spectrum shows the absorption bands of Gd-O, Y-O and Mo-O respectively. Particle size calculated from TEM shows a good agreement with the X-ray data. UV-Vis spectrum shows the prepared material have a direct bandgap with bandgap energy of 3.45eV.

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