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SDC Journal of Theoretical and Experimental Research (SDCJTER) 01(02), 2023, 13–18

A study on Structural and Optical properties of $Sr_3(VO_4)_2$ ceramic

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Available online 01 June 2023

Abstract

$Sr_3(VO_4)_2$ ceramic has been synthesized using conventional solid state reaction method. The structural and optical properties of synthesized ceramic done using X-ray diffraction (XRD), Fourier Transform Infra-Red spectroscopy (FTIR) and UV-Visible absorption spectroscopy. XRD analysis reveals that the synthesized ceramic exists in single phase with rhombohedral structure. The space group is R-3m (166) with lattice parameters a = 5.6197(2) Å and c = 20.103(2) Å. It possess centro-symmetric in crystal structure. The various vibrational bands present in the $Sr_3(VO_4)_2$ ceramic are identified from FTIR study. The electronic transitions and optical band gap of the ceramic is recorded from UV- Visible spectrum. The ceramic has a direct band gap of 3.23 eV. The synthesized orthovanadates has peculiar role in the field of light emitting diodes, solid state lighting and photocatalytic purposes.

Keywords: Citation Analysis, Mars, Martian Atmosphere, Life, Dust Storms, GCM

1. Introduction

Vanadates have attracted much attention because of their rich structural chemistry which easily adapts to various structural forms like tetrahedral, square-pyramidal and octahedral coordination environments in various oxidation states [1]. They find applications in a wide range of industries and continue to be of interest for their unique properties and potential contributions to technology and science. Vanadium oxide compounds are widely used as luminescent indicators, thermo luminescent detectors, scintillators etc [2].Vanadates are the subject of ongoing research in fields such as materials science, chemistry, and catalysis. Scientists are exploring novel vanadate compounds and their applications, particularly in renewable energy and environmental remediation. Based on the structural difference between the vanadium-oxygen units, vanadates can be classified as pyrovanadate, orthovanadate and metavanadate [3]. The alkaline earth metal orthovanadates with general formula, $M_3(VO_4)_2$ (M = Ca, Sr, Ba). In orthovanadates, vanadium is in its highest oxidation state, which is +5. This high oxidation state imparts specific chemical properties to orthovanadate compounds. This compounds have received a lot of attention for possible uses in nanophotonics, IR laser systems, light-emitting diodes, photocatalysis, ferroelectric and microwave devices [4].

2. Experimental techniques

2.1 Sample preparation

$Sr_3(VO_4)_2$ ceramic was synthesized by conventional solid-state reaction method. The stoichiometric amounts of $SrCO_3$ (99.6%, Sigma Aldrich) and Vanadium pentoxide (V_2O_5) were used as starting materials. The required stoichiometric amounts of these raw materials were weighed accurately and then thoroughly mixed in an

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agate mortar and pestle with distilled water as the medium for 2 hours. It was then dried in an oven and then transferred into a platinum crucible and calcined at an optimum temperature of 625^0 C for 4 hours at a heating rate of 10^oC/min. The calcined powder was then again ground well for characterization.

2.2 Characterization techniques

The phase identification of the synthesized ceramic was done with X-ray diffraction technique on powder samples using a Bruker AXS D8 Advanced X- ray diffractometer. The pattern was collected over the 2θ in the range 10-80 degrees. The Fourier transform infrared spectrum of the synthesized ceramic was recorded in the range of 400 - 4000 cm^{-1} using PerkinElmer FTIR/ FIR Spectrometer. The regions of absorptions and band gap energy of the ceramic was determined from UV-Visible studies using PerkinElmer UV/VIS/NIR Spectrometer Lamda 950 in the range 200 - 800 nm.

3. Results and Discussions

3.1 X-Ray Diffraction (XRD)

XRD patterns of $Sr_3(VO_4)_2$ ceramic is shown in Figure 1. All the diffraction peaks of the synthesized phosphor are in good agreement with standard ICDD card no. (00-029-1318). The structure of the ceramic is rhombohedral with space group R-3m (166). The lattice parameter is a = 5.6197(2) Å and c = 20.103(2) Å. It possess centro-symmetric in crystal structure [5-7].

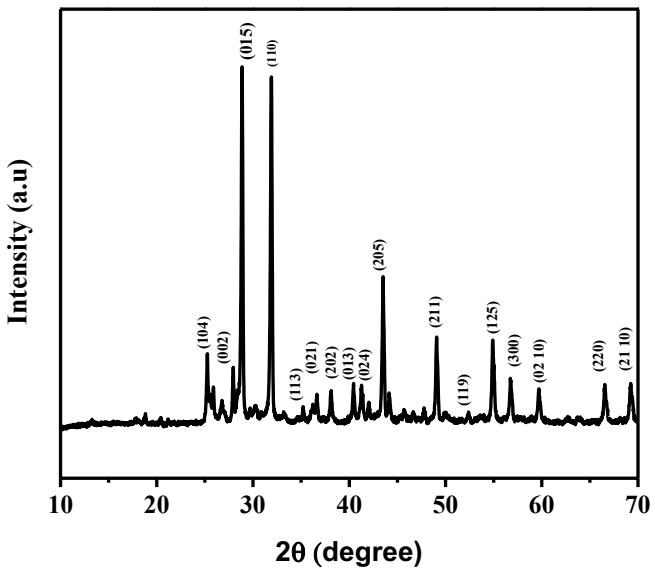

Figure 1 XRD pattern of Sr3(VO4)2 ceramic

3.2. Fourier transform infrared spectrum (FTIR)

The Fourier Transform Infra-Red spectroscopy (FTIR) provides the characteristics of the elements and vibrational bands present in the ceramic. FTIR spectrum of $Sr_3(VO_4)_2$ ceramic is shown in **Figure 2**. The prominent bands are recorded at 610, 811, 895, 1117 and 14667 cm^{-1}. The band assigned at 610 cm^{-1} corresponds to the Sr-O bending vibrations [8]. In most cases intense peaks in the 550 - 950 cm^{-1} region attributed to several M-O stretching and bending vibrations of the VO_4^{3-} group [9]. V-O stretching vibration bands exist in the region 800 - 950cm^{-1} [7].

Modes in the region 700 – 1250 cm $^{-1}$ are due to $(VO_4)_2$ absorption bands, which are assigned to the O–V–O bending vibrations and V–O stretching vibrations, respectively [6]. The peak assignments in the range of 1300 –1800 cm $^{-1}$ are attributed to the absorption of the H–O–H bending vibrations [10].

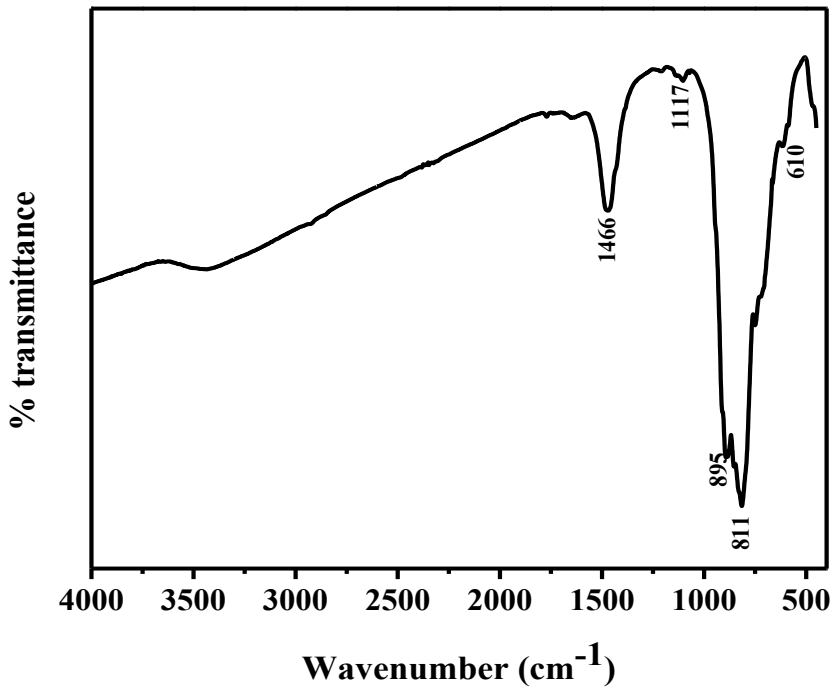

Figure 2 FTIR spectrum of Sr3(VO4)2 ceramic

3.3 UV-Visible studies

The optical absorption measurement is one of the important factors for the determination of band structure as well as the band gap energy of the synthesized $Sr_3(VO_4)_2$ ceramic []. **Figure 3(a)** represents the UV-Visible absorption spectrum of $Sr_3(VO_4)_2$ ceramic. The absorption spectrum reveals that the maximum absorption of host occurs in the range 250 – 300 nm. After 300 nm absorption tailoring occurs [11].

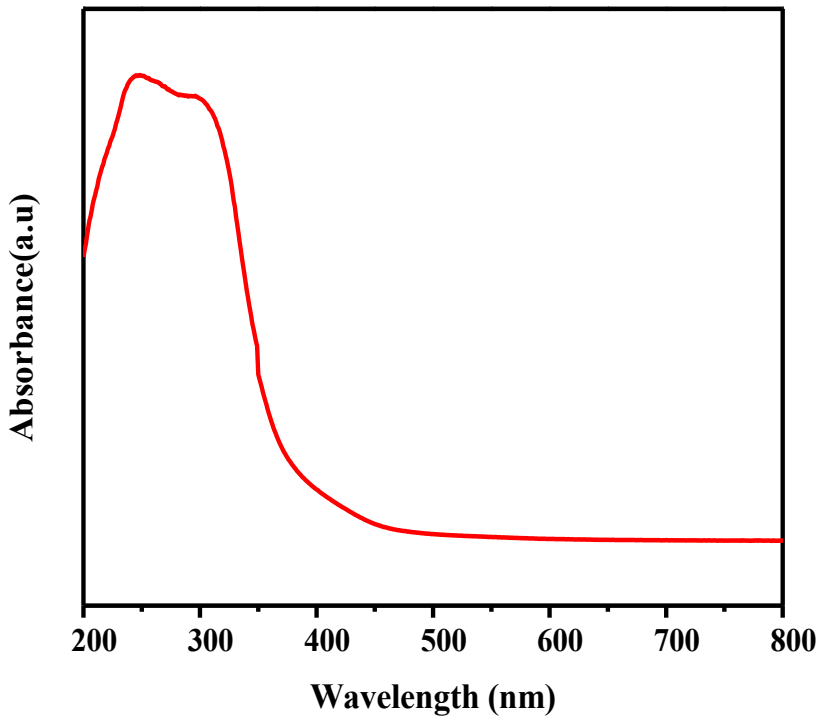

Figure 3(a) Absorption spectrum of Sr3(VO4)2 ceramic

Figure 3(b) represents the direct band gap energy of $Sr_3(VO_4)_2$ ceramic. The band gap energy of a material describes the energy required to excite an electron. The energy - dependent absorption coefficient α can be expressed by the Tauc method using the equation

$$(\alpha h\nu)^{1/n} = c\,(h\nu - E_g) \qquad (1)$$

Where hν is the photon energy and α is the absorption edge, the value of α is obtained from absorption spectra, E_g is the band gap energy and c is a constant. The value of n depends on the nature of the electron transition and is equal to 1/2 for the direct allowed transitions. The direct band gap is estimated to be 3.23 eV [8, 11].

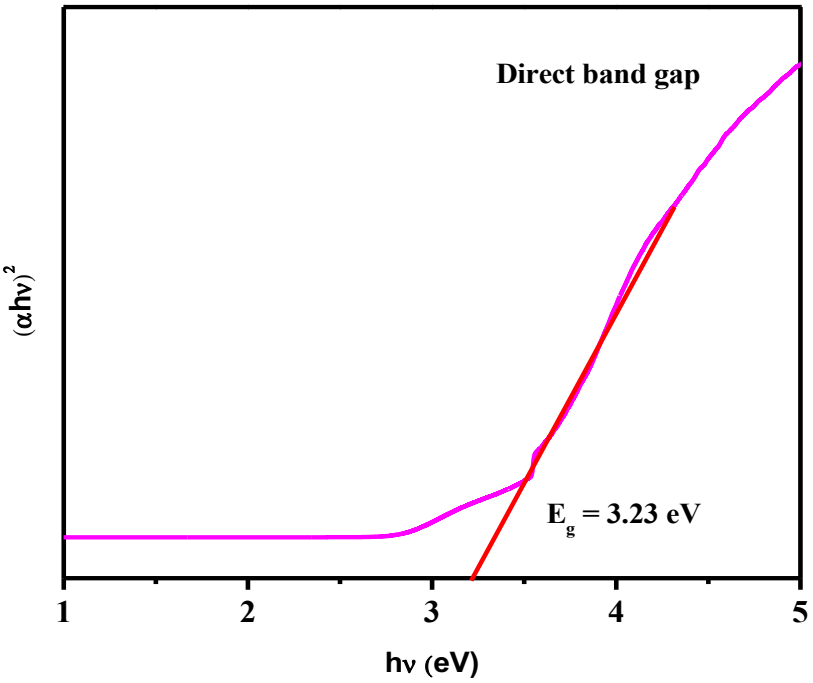

Figure 3(b) Direct band gap energy of Sr3(VO4)2 ceramic

4. Conclusions

$Sr_3(VO_4)_2$ ceramic has been synthesized using solid state reaction method. The structural and optical properties of prepared ceramic calcined at 650^0 C are investigated. XRD pattern reveals that it is rhombohedral in structure with space group R-3m (166). The lattice parameter is a = 5.6197(2) Å and c = 20.103(2) Å. FTIR analysis confirms the vibrational modes present in the ceramic. The region of absorption and direct band gap energy of the ceramic is estimated from UV-Visible absorption spectrum. The direct band gap energy is calculated to be 3.36 eV.

Acknowledgments

The authors are thankful to the Department of Physics, Kariavattom Campus for the X-ray diffraction studies and FTIR facility. The authors are grateful to the Department of Optoelectronics, Kariavattom for UV-Visible characterization.

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