Section A-Research paper
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Synthesis of V_2O_5 with Acid Blue 9 molecules for Optoelectronic Device Applications

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Abstract

Vanadium pentoxide (V2O5) with organic dye acid blue 9 molecule was synthesized using precipitation method with distilled water as solvent. The synthesized powdered sample was characterized by Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR), UV-vis-NIR spectroscopy and Photoluminescence spectroscopy analyses. PXRD pattern shows that the synthesized sample was in the micro rod like structure. SEM picture informs the morphology of the synthesized sample as in micro rod-shaped structure. The UV-vis- NIR absorption spectrum shows an absorption band at 245 nm which is the cut off wavelength of the synthesized powder sample and to confirm dielectric nature. The photoluminescence spectrum exhibits infrared light at Eg=1.62 eV due to V2O5 molecule levels located inside the band gap along with acid blue 9 molecule. The calculated dielectric values of the sample V2O5 and synthesized sample were 0.44 and 0.55 which imply the dielectric nature of synthesized sample.

Keywords: Powder XRD, Luminescence, Optical materials, Dielectrics.

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1. Introduction

Vanadium oxide is a well-known catalyst among various metal oxides, and so many fundamental studies have been developed for wide-spreading centering on catalytic oxidation. They show metal-semiconductor transition, which implies an abrupt change in optical and electrical properties. That is why V2O5 is used in thermal sensing and optical switching devices. Vanadium pentoxide-based materials are known to display several types of chromogenic effects, as a window for solar cells and for transmittance modulation in smart windows with potential applications in architecture, automotives and nanomedicine. It shows a typical behavior because it cannot be defined exactly either as a cathodically or as anodically coloring material. V2O5 material exhibits multi-colored electrochromic allowing the use in electrochromic (EC) displays color filters and other optical devices [1]. Electroluminescence of organic molecules has been a well-known phenomenon since the mid twentieth century. However, it was not until 1987 that organic light-emitting diodes (OLEDs), sometimes called organic light-emitting devices, became promising for practical applications, when Tang and Van Slyke demonstrated the first high-efficiency devices. OLEDs are unique technology, based on the use of organic molecules to conduct large amount of charge, which recombines to emit light that is bright enough for displays or general lighting devices. Successful application of organic luminescence of light-emitting devices required materials and devices structures that overcame the intrinsically high resistivity of the organic materials while achieving balanced charge injection from electrodes into organics [2]. In this research work, the synthesis of V_2O_5 molecule with acid blue 9 dye molecule was done and the corresponding characteristics such as powder XRD and SEM analysis were carried out for the conformation of the micro rod structure. The presence of the molecular vibration in the synthesized material was assigned using FTIR spectral analysis. The optical properties were observed using UV-vis-NIR spectral and photoluminescence analyses. Photoluminescence (PL) is an optical phenomenon exhibited by some semiconductor materials when excited by an electromagnetic radiation source [3]. The advantages of PL analysis listed above derive from the simplicity of optical measurements and the power to probe fundamental electronic properties [4]. The increasing value of dielectric constant for the synthesized V2O5 with acid blue 9 molecule was calculated using dielectric constant apparatus (for solid and liquid).

2. Experimental Method

Precipitation method was used for the preparation of the sample. The process was initiated by mixing with 2.1 g of V2O5 and 7.9 g of acid blue dye in the ratio of 1:1 respectively with the water as solvent. The mixture was stirred for 10 hours at room temperature. The solution was filtered and was allowed to collect the powder sample. The filtered residue was annealed and dried at 450**°C** for 24 hours using hot air oven. The photograph of the dried powder sample is shown in Fig 1.

Fig 1. Photograph of the dried powder sample

3. Results and Discussion

3.1. Powder XRD analysis

X-ray diffraction (XRD) is a widely used technique to assess the crystalline nature and structure of solid samples. In summary, the crystal X-ray diffraction phenomenon results from a scattering process in which X-rays are scattered by the electrons of atoms present in the sample without changing the wavelength. The resulting diffraction pattern, given by the position and intensities of the diffraction effects, is a fundamental physical property of the material, providing not only the identification but also the complete elucidation of its structure [5]. Powder X-ray diffraction (PXRD) measures the diffraction pattern of crystalline material [6]. Powder XRD analysis of the prepared sample can be measured using CuKα radiation source ($\lambda = 1.54050$ Å). The PXRD pattern of the synthesized V2O5 with acid blue 9 molecules which was annealed at

450 °C is shown in Fig 2. The PXRD patterns of powdered sample were recorded by scanning 2θ and intensity that gives a greater number of peaks which denotes the micro rod like structure.

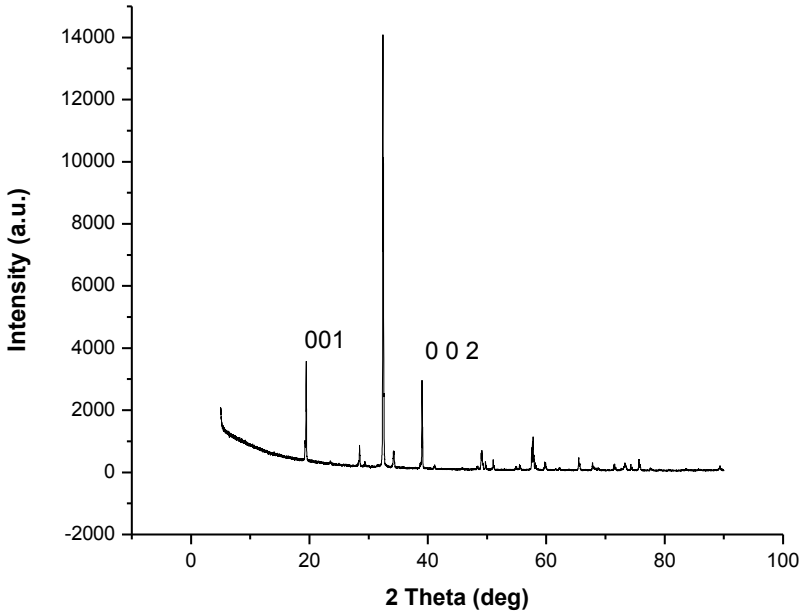

Fig 2. PXRD spectrum of the sample

3.2. SEM analysis

The Scanning Electron Microscope (SEM) is routinely used to study the surface structure and chemistry of a wide range of biological and synthetic materials at the micrometer to nanometer scale. Ease-of-use, typically facile sample preparation, and straight forward image interpretation, combined with high resolution, high depth of field, and the ability to undertake micro chemical and crystallographic analysis, has made scanning electron microscopy one of the most powerful and versatile technique for characterization today [7]. Scanning electron microscopy (SEM) uses a focused beam of high-energy electrons to create a variety of signals on the surface of solid samples. The SEM is also capable of carrying out analyses of chosen points on the sample. This approach is particularly useful for the qualitative or semi-quantitative determination of chemical compositions, crystalline structure, and crystalline orientation [8]. The SEM analysis of the prepared sample can be measured using the Carel Zeiss Instrument. SEM studies were carried out for pure V2O5 and for the mixture of V2O5 and acid blue 9 molecules to obtain information on the morphology of the prepared sample. It also indicated high porosity on the sample surface when the annealing temperature was increased. The morphology of the synthesized sample was

observed in micro rod shape when the temperature was increased to 450 °C. The SEM image of the sample is annealed at 450 °C and is shown Fig 3a and 3b. The observed value of the pure V2O5 be 116 nm and 140 nm and for V2O5 with acid blue 9 molecules is 147 nm, 148 nm and 139 nm which is in micro-rod like shape. It is concluded that the thickness of the pure V2O5 particle is changed by adding the dye molecules into it for improving the optical properties of V2O5 molecules. This tunability of the size of the vanadium pentoxide and their multivalent nature will help in its various applications where specific dimensions of the rods are required and in electrochemical applications, catalysis etc. [9].

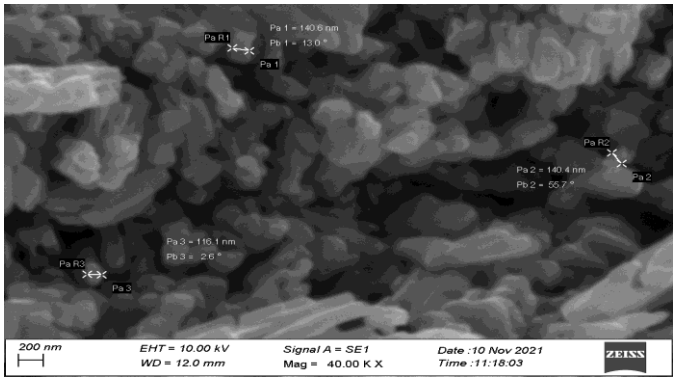

Fig 3a. SEM image of pure V_2O_5

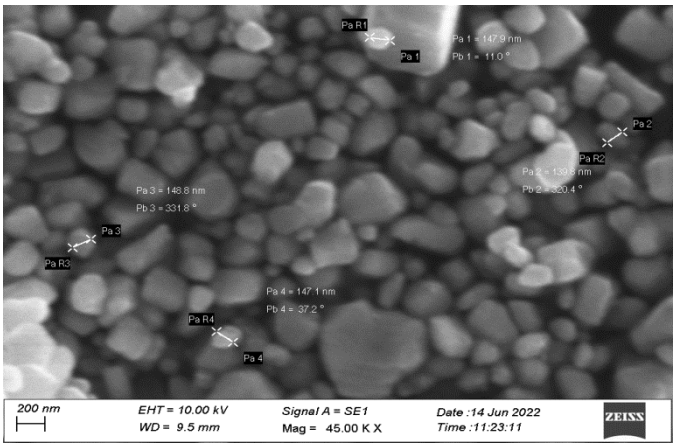

Fig 3b. V_2O_5 with acid blue 9 molecule

3.3. FTIR Spectroscopy analysis

Fourier transform infrared spectroscopy (FTIR) is a technique used to identify the functional groups in the materials (gas, liquid, and solid) by using the beam of infrared radiation [10]. IR

vibration spectroscopy is a technique that can be utilized to identify molecules by analyzing their constituent bonds. Each chemical connection of a molecule vibrates at a specific frequency. A group of atoms in a molecule (such as CH_2) can have several modes of oscillation caused by the stretching and bending movements of the molecules as a whole [11]. An infrared spectroscopy measured the absorption of IR radiation made by each bond in the molecule and as a result gives spectrum which is commonly designated as % transmittance versus wavenumber (cm 1). The FTIR spectrum of the prepared sample can be recorded by using the instrument called Perkin Elmer Spectrum FTIR Spectrophotometer. FTIR spectrum can be taken in the range from 4000 cm^{-1} to 400 cm^{-1}. The FTIR spectral analysis of the sample is shown in Fig.4. It is observed that the wave numbers of 3452 cm^{-1} indicates the presence of N-H group of acid blue 9 molecules. The peaks at 2992 cm^{-1} and 2249 cm^{-1} correspond to the presence of stretching modes of C=N molecule, at 1638 cm^{-1} assigned C=O of COOH and at 1124 cm^{-1} corresponds to the S=O stretching of organic acid blue 9 dye molecule. The peak at 616 cm^{-1} corresponds to the presence of vanadium material and vanadium pentoxide molecules. The FTIR assignment of synthesized sample is shown in Table 1 confirms the chemical structure of the synthesized sample with V_2O_5 and organic acid blue 9 molecules.

Table 1. FTIR assignment of synthesized sample

Wave number (cm^{-1})	**Assignment**
3452	N-H
2992	N-H
2249	C=N
1638	C=O
1124	S=O
616	V-O-V

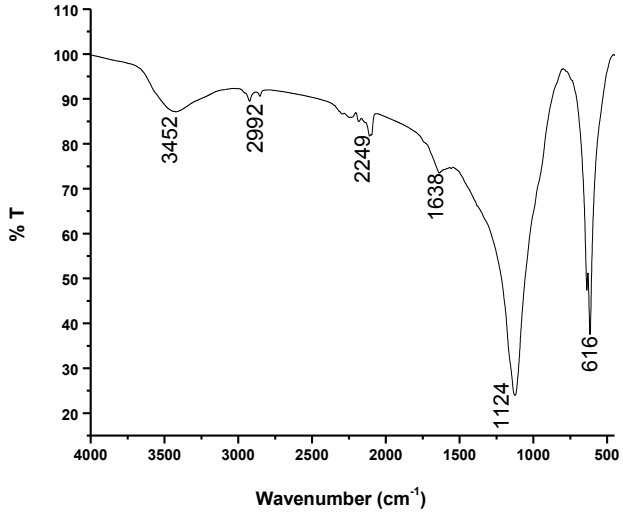

Fig 4. FTIR spectrum of the sample

3.4. UV vis Spectroscopy analysis

Ultraviolet/visible (UV/VIS) absorption spectroscopy is a powerful yet cost-effective tool that is widely used to identify organic compounds and to measure the concentration of principal and trace constituents in liquid, gas, and solid test samples [12]. The absorbance in the visible area influences the color of the sample and undergoes electron transitions. Absorbance is directly proportional to the path length "b" and concentration of the sample "c." UV spectroscopy obeys the Beer-Lambert law, which states that: when a beam of monochromatic light is passed through a solution of an absorbing substance, the absorbance is directly proportional to the log values of the ratio between the intensity of light incident upon sample cell and the intensity of light leaving the sample and aso directly proportional to it molar concentration of solute. A = log10 (I0/I) ϵCL, where A is absorbance, I0 is intensity of light incident upon sample cell, I is the intensity of light leaving sample cell, C is molar concentration of solute, L is length of sample cell (cm) and ϵ is molar absorptive [13]. The UV-vis-NIR spectral study of the sample can be recorded using Varian Cary SE UV-vis-NIR Spectrophotometer. The UV-vis-NIR Spectrum of the sample can be taken in the range from 100 nm to 1000 nm as shown in Fig.5. The Cut off wavelength of the prepared sample is found as 245 nm as shown in Fig 5. The corresponding value of energy gap is determined by using the formula Eg = hc/λc, where λc be the cut off wavelength, h be the Planck's constant and c be the velocity of light. From this formula, the value of energy gap will

be calculated as 5.06 eV. The calculated band gap value of the sample shows that the sample belongs to insulating materials. Hence the synthesized sample is the promising material for optoelectronic devices.

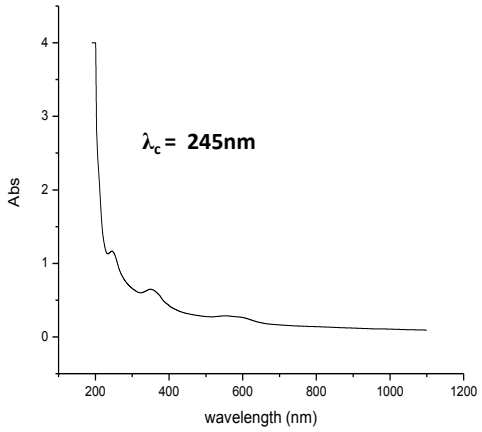

Fig 5. UV vis NIR spectrum of the sample

3.5. Photoluminescence (PL) analysis

Photoluminescence (PL) analysis is used to investigate the separation of photo generated charge carriers because the PL signal resulted from recombination of photo generated electron-hole pairs [14]. The PL spectral study can be recorded using the instrument called Perkin Elmer LS 45. The Photoluminescence measurement of V_2O_5 with acid blue 9 molecule was carried out and the graph is shown in Fig 6. The photoluminescence analysis of pure V_2O_5 centered by the Gaussians peak at λ =400 nm which is bluish green region [15], after adding acid blue 9 dye molecules the particle emitted infrared light that was fitted by one Gaussians peaks centred at emission band at λ =436 nm in bluish green region and λ=764 nm corresponding to photon energy of E_g=1.62 eV shows the largest wavelength which is red region. Thus, the adding of acid blue 9 dye molecule with v205 material improves its possibility for OLED applications. This band gap energy suggests that V_2O_5 with acid blue 9 dye molecule levels are located inside the band gap along with acid blue 9 molecules [16], which is in good agreement with optical absorption measurement. So, the synthesized V_2O_5 and acid blue 9 molecule is a promising material for the application of opto-electronic devices [17].

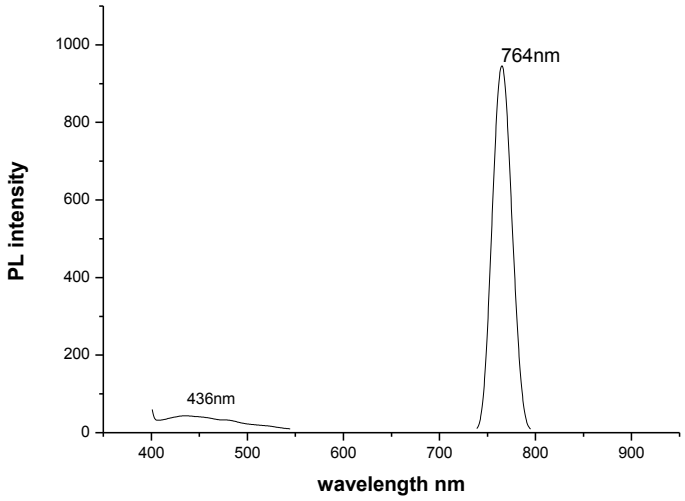

Fig 6. Photoluminescence spectra of V_2O_5

3.6. Dielectric Studies

The study of dielectric properties concerns storage and dissipation of electric and magnetic energy in materials [18]. Dielectrics are important for explaining various phenomena in electronics, optics, solid-state physics and cell biophysics [19]. Dielectrics -are such a media that can store, not conduct, electrical energy. A measure for this property is the permittivity or dielectric constant of the material. Infact, permittivity is only a higher-level invention to calculate the electric response of matter [20]. The dielectric study can be measured using the instrument called Dielectric Constant Setup (for Solid and Liquid) and the setup can be shown in Fig 7. The measured dielectric constant value of V_2O_5 and synthesized V_2O_5 with acidic blue 9 molecule were obtained as 0.44 and 0.55 by calculated using the formula $\mathbf{K}=\frac{C_1-C_2}{C_1-C_3}$. The calculated dielectric value of the sample shows that organic acid blue 9 molecule improves the dielectric constant of V_2O_5 molecule. Hence by increasing the value of dielectric constant of the sample, it understood that the synthesized V_2O_5 with acid blue 9 molecules is suitable component for opto-electronic devices.

Fig 7. Dielectric Constant Setup

4. Conclusion

The synthesized V_2O_5 with acid blue 9 molecules were successfully prepared with distilled water as solvent using precipitation method. By varying sample temperature on the evolution of structure (at T = 450 °C), micro rod structure of synthesized sample was investigated. The micro rod nature of the synthesized powdered sample was determined using Powder XRD analysis. The SEM image shows rod-like shape and the thickness of pure V_2O_5 increased by adding acid blue 9 molecules. The presence of V_2O_5 molecule and acid blue 9 molecules in the synthesized powder sample was confirmed using FTIR analysis. The UV-vis- NIR absorbance spectrum of the sample was observed within the range of 100-1000 nm which illustrates the insulating nature of the sample with the calculated energy gap value as 5.06 eV. A broad photoluminescence peak around 436nm and 764 nm were studied using Perkin Elmer LS 45. Additionally, the synthesized sample has been found to have increased dielectric nature. From these optical studies, it is confirmed that the synthesized V_2O_5 and acid blue 9 molecule is a promising material for the application of optoelectronic devices.

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