

Characteristic Studies of 2D Materials PVA Augmented by Vanadium Oxide

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Abstract : Blends of vanadium pentoxide (V_2O_5) and polyvinyl alcohol (PVA) have attracted significant interest for their potential applications in electrochemical devices, sensors, batteries, and optical coatings. V_2O_5 , a transition metal oxide with semiconducting and catalytic properties, enhances the thermal stability, conductivity, and mechanical strength of PVA, a flexible, water-soluble polymer. The structural and morphological characteristics of these composites are often analysed using FTIR spectroscopy. The blend exhibits strong UV-visible absorption, making it suitable for photodetectors and optical coatings. V_2O_5 doping improves PVA's electrical conductivity, enabling applications in electrochemical energy storage, including lithium-ion and sodium-ion batteries, supercapacitors, and solid-state electrolytes. Additionally, PVA- V_2O_5 composites contribute to electrochromic devices for smart displays and windows, leveraging V_2O_5 's ability to undergo color changes under applied voltage. This study highlights the multifunctionality of PVA- V_2O_5 composites and their potential for next-generation energy and sensing technologies.

Keywords-Electrochemical devices, sensor, optical, composite, electrochromic devices.

Introduction - Two-dimensional (2D) materials have attracted significant research interest due to their remarkable electrical, optical, and mechanical properties, making them promising candidates for next-generation electronic, sensing, and energy-storage applications [1]. Among these materials, transition metal oxides (TMOs) such as vanadium pentoxide (V_2O_5) are particularly noteworthy due to their ability to exist in multiple oxidation states, a result of their half-filled d-orbitals. This characteristic enhances their catalytic and electronic properties, enabling their use in applications ranging from semiconductors and photovoltaics to electrodes and environmental sensors [2-4]. However, despite their advantages, many 2D materials face challenges related to structural stability, mechanical flexibility, and processability, which limit their widespread adoption.

To address these limitations, researchers have focused on integrating TMOs with polymeric matrices to develop novel composite materials with enhanced functionality. Polyvinyl alcohol (PVA) has emerged as a suitable polymer for this purpose due to its excellent film-forming ability, mechanical flexibility, biocompatibility, and environmental friendliness. The incorporation of V_2O_5 into a PVA matrix offers a unique approach to developing hybrid materials with improved conductivity, mechanical integrity, and stability while maintaining flexibility [5-7]. These PVA- V_2O_5 composites hold significant potential for various

applications, including electrochemical sensing, photodetection, and energy-efficient coatings [8].

Fourier Transform Infrared (FTIR) spectroscopy is a powerful analytical technique used to study the structural and chemical interactions within composite materials. In the case of PVA- V_2O_5 composites, FTIR spectroscopy provides crucial insights into the bonding mechanisms, phase interactions, and functional group modifications that occur during the blending process. The analysis of characteristic vibrational modes helps in understanding how V_2O_5 interacts with PVA at the molecular level, influencing the material's overall properties. The study of these interactions is essential for optimizing the composite's electrical, optical, and mechanical behaviour.

Electrochemical sensors based on 2D nanomaterials have been extensively studied for detecting environmental contaminants such as heavy metals, toxic gases, organic pollutants, pesticides, and bacteria [9-11]. The incorporation of V_2O_5 into PVA-based composites can enhance sensor sensitivity, selectivity, and stability, making them promising candidates for industrial safety and environmental monitoring. Additionally, V_2O_5 is strong UV-absorbing properties, when combined with PVA, enable the development of advanced optical coatings and flexible photodetectors for UV-visible light detection, which can be incorporated into wearable sensors and optoelectronic devices.

Beyond sensing applications, PVA- V_2O_5 films exhibit potential in biomedical applications due to their antibacterial properties, making them suitable for coatings on medical devices, wound dressings, and controlled drug release systems [12]. Furthermore, the integration of these composites into flexible electronics enables their use in transparent conductive films, thin-film transistors, and electrochromic displays, where mechanical flexibility and electrical conductivity must be balanced.

The goal of the current study is to offer some information on new compounds that are expected to be easily exfoliable from a parent bulk molecule and have anisotropies that significantly outperform those of previously found 2-dimensional substances [13,14]. The findings of this study will be a comprehensive guide for future research on anisotropic response in thin crystals and will highlight opportunities and challenges for the creation of gauges based on two-dimensional materials [15,16].

This research investigates the physicochemical properties of PVA- V_2O_5 composites, with a particular focus on their structural, electronic, and magnetic characteristics. By utilizing FTIR spectroscopy, we aim to analyse the molecular interactions and bonding changes that contribute to the enhanced properties of these composites. Additionally, this study explores how the integration of V_2O_5 with PVA can improve the electrical performance of 2D materials, contributing to advancements in high-performance electronic, optical, and sensing technologies. The findings will provide valuable insights into the design and development of novel anisotropic 2D materials and their potential applications in flexible electronics, environmental monitoring, and biomedical engineering.

Materials and Methods: Vanadium pentoxide (V_2O_5), PVAc with the medium molecular weight of 86.09 g mol^{-1} , were obtained from Merck Chemical Co. (Germany). Sodium hydroxide (NaOH), Hydrochloric Acid (HCl), was acquired from Sigma-Aldrich (Germany). Ethanol and distilled water were attained from local market.

Preparation of Poly Vinyl Alcohol solution: Exactly 1 gm of Polyvinyl acetate (PVAc) is dissolved in a mixture of ethyl alcohol and distilled water around 30ml. The temperature has been maintained at around $60-80^\circ\text{C}$ to ensure proper dissolution. The solution stirred continuously to achieve a homogeneous mixture. A measured amount of sodium hydroxide solution has been added to the PVAc solution. The catalyst facilitates the hydrolysis (saponification) of PVAc into PVA and acetic acid. The reaction mixture has been maintained at $60-80^\circ\text{C}$ and stir continuously. The reaction progress monitored. Partial hydrolysis yields partially hydrolyzed PVA, while complete hydrolysis produces fully hydrolyzed PVA. Once the desired degree of hydrolysis is achieved, the reaction mixture has been neutralized by adding a weak acid (e.g., acetic acid or hydrochloric acid). This step prevented further reaction and stabilizes the PVA solution. The PVA precipitated by

pouring the reaction mixture into a large volume of cold water. The PVA precipitate has been collected by filtration or centrifugation. The precipitate washed multiple times with water to remove residual catalysts and by-products. The washed PVA dried under in an oven at a low temperature ($50-70^\circ\text{C}$) until a constant weight is achieved [17].

Preparation of PVA- V_2O_5 composite: Exactly 1g of PVA dissolved in 30 ml of distilled water. The temperature has been maintained at around $60-80^\circ\text{C}$ to ensure proper dissolution. The solution stirred continuously to achieve homogeneous mixture. In another beaker 0.1 g of V_2O_5 is dissolved in minimum quantity of H_2SO_4 by continuous stirring at room temperature until orange homogenous solution was obtained. Then V_2O_5 solution was added dropwise to PVA solution with continuous stirring for 2-3 hr, solution color turns to lemon green. The reaction temperature is maintained between $60-80^\circ\text{C}$. A black color precipitate starts to appear of PVA- V_2O_5 composite then later filtered with Buchner funnel using vacuum pump, washed 2-3 times with distilled water and left for complete drying in air for 2-3 days. A black amorphous solid of PVA- V_2O_5 was obtained.

Results and Discussion: The incorporation of V_2O_5 into PVA results into enhancement in several properties of polymer. The FTIR spectrum provides insights into the chemical bonding, structural changes, and interactions between PVA and V_2O_5 . Additionally, FTIR spectroscopy has been employed to identify the functional groups present in the synthesized compounds.

The Table 1 shows the most characteristic bands of PVA and their respective assignment. Fig.2 shows the FTIR spectra of PVA. All major peaks related to hydroxyl group were observed. The large bands observed between 3550 and 3200 cm^{-1} are linked to the stretching O-H from the intermolecular and intramolecular hydrogen bonds (Fig.2). The vibrational band observed between 2840 & 3000 cm^{-1} refers to the stretching C-H from alkyl groups (Fig.2) and the peaks between $1750-1735 \text{ cm}^{-1}$ (Fig.2) are due to the stretching C=O and C=O from acetate group remaining from PVA [17].

The FTIR spectra to PVA crosslinked with V_2O_5 is presented in Fig.3. The reaction of the PVA with the V_2O_5 results in a considerable reduction of the intensity of the O-H peaks (in Fig.3) from the composite, indicating a possible formation of acetal bridges. For instance, FTIR spectra of PVA- V_2O_5 samples (Fig.3) reveal bands at ($\nu=3090-2990 \text{ cm}^{-1}$) signifies the C-H stretching, (Fig.3) a duplet absorption with peaks attributed to the alkyl chain. Also, strong band from carbonyl group was verified (C=O at $\nu=1677-1685 \text{ cm}^{-1}$). These bands are overlapping and broadening PVA bands in these regions. In addition to that, by crosslinking PVA with V_2O_5 , the O-H stretching vibration peak ($\nu=3250-3450 \text{ cm}^{-1}$) was relatively decreased when compared to pure PVA. Stretching vibration peak ($\nu=1143 \text{ cm}^{-1}$) for C-O crystallinity. C-O-C stretching vibration peak

($\nu=1038-1073\text{ cm}^{-1}$) which remained almost constant. CH_2 Bending vibration peak ($\delta=1384\text{ cm}^{-1}$) which is constant. Polymer composite show the same pattern with additional stretching bands at ($\nu=400-600\text{ cm}^{-1}$) which is due to V_2O_5 vibrations [18]. It is apparent from the fig.3 that the intensity of peaks is getting decrease with addition of V_2O_5 . It is due to the compatibility of V_2O_5 with polymer.

Figure 1.FTIR spectra of V_2O_5

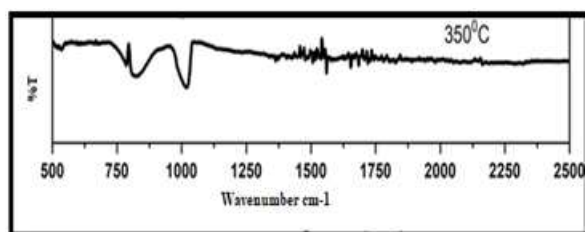


Figure 2.FTIR spectra of PVA

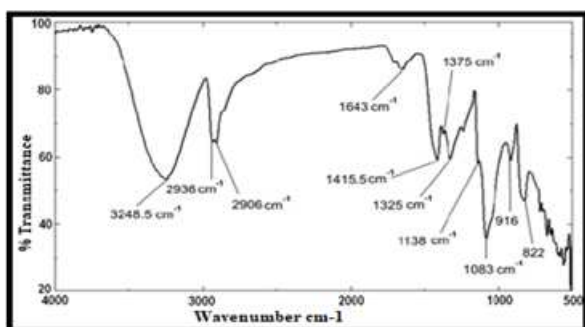


Figure 3. FTIR Spectra of PVA- V_2O_5 (Original)

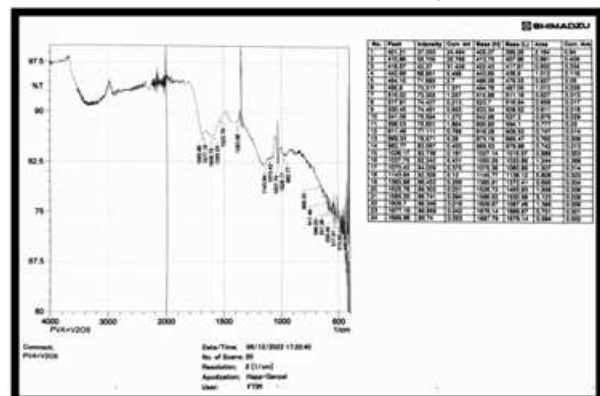


Table 1:FTIR of PVA- V_2O_5 (extracted)

No.	Peak	Intensity	Corr. Int
1	401.21	37.055	24.494
2	410.86	55.705	25.768
3	418.57	42.37	31.428
4	442.68	66.951	5.488
5	484.15	71.685	2.7
6	490.9	73.317	1.371
7	515.02	73.305	1.037
8	517.91	74.427	0.213
9	530.45	74.491	0.853
10	541.06	75.594	1.272
11	596.03	75.601	1.864

12	611.46	77.111	0.769
13	669.33	79.571	0.28
14	982.77	83.587	0.453
15	1026.17	82.738	0.181
16	1037.75	82.242	5.431
17	1073.43	84.029	0.375
18	1143.84	82.308	0.12
19	1363.98	88.453	0.259
20	1525.76	89.303	0.131
21	1585.65	87.741	0.094
22	1609.87	86.346	0.08
23	1677.18	86.859	0.042
24	1685.86	86.74	0.053

Conclusion and Future Scope: The incorporation of vanadium pentoxide (V_2O_5) into polyvinyl alcohol (PVA) matrices results in multifunctional composite materials with enhanced mechanical strength, thermal stability, and electrical conductivity. These composites exhibit significant potential for various applications, including electrochromic smart windows, energy-efficient coatings, flexible photodetectors, and biomedical coatings. The PVA- V_2O_5 films also demonstrate high sensitivity to environmental gases such as humidity, ammonia (NH_3), and nitrogen dioxide (NO_2), making them suitable for industrial safety and environmental monitoring. Additionally, the antibacterial properties of PVA- V_2O_5 composites enable their use in wound dressings and medical device coatings, with the potential for controlled drug release applications.

FTIR spectroscopy has been instrumental in analysing the chemical interactions and bonding mechanisms within these composites, providing valuable insights for optimizing their properties. The results highlight the role of V_2O_5 in significantly improving the physicochemical characteristics of PVA, where the degree of enhancement is influenced by factors such as particle size, concentration, and dispersion within the polymer matrix.

Further studies can focus on optimizing the size, concentration, and distribution of V_2O_5 particles within the PVA matrix to achieve superior mechanical, optical, and electronic properties. Advanced surface modifications and functionalization techniques can be explored to enhance the compatibility of V_2O_5 with PVA. Investigating the potential of PVA- V_2O_5 composites as electrode materials for supercapacitors and lithium-ion batteries. Exploring their role as solid polymer electrolytes to improve ionic conductivity and battery cycle life. Enhancing the sensitivity and selectivity of PVA- V_2O_5 composites for detecting toxic gases and pollutants in environmental applications. Integration into flexible and wearable sensor devices for real-time monitoring. Expanding research on the biocompatibility and antimicrobial efficiency of these composites for advanced wound healing and infection control. Studying their potential for controlled drug release in targeted therapy. Developing high-performance optical coatings, UV-blocking films, and flexible photodetectors for

wearable electronics. Investigating the potential of these composites in smart windows and electrochromic display technologies.

By addressing these research directions, the PVA- V_2O_5 composite system can be further refined for widespread adoption in various industrial, environmental, and biomedical applications, paving the way for next-generation functional materials.

Conflict of Interest: The writers have indicated that they have no conflicts of interest.

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