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**SYNTHESIS AND CHARACTERISATION OF MOLYBDENUM
DISULPHIDE-BORON NITRIDE (MO₂-BN) COMPOSITE FOR
WATER TREATMENT APPLICATIONS**

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ABSTRACT

Water scarcity and pollution have emerged as a critical global challenge, which makes a necessity to the development of advanced materials for efficient water treatment. Significant focus has been placed on two-dimensional these materials possess unique properties due to their ultrathin structure, large surface area, and exceptional mechanical, electrical, and chemical properties. Boron nitride(BN) is the material which is mostly used, BN sheets can be fabricated into membranes for water filtration. BN membranes possess high mechanical strength, thermal stability, and excellent chemical inertness. It exhibits a high surface area and chemical stability, making them promising adsorbents for water purification. MoS₂ is a two-dimensional nanomaterial with a layered structure, similar to graphene. MoS₂ exhibits photocatalytic properties under light irradiation, enabling the degradation of organic pollutants and disinfection of water and in electrocatalysis, it can facilitate the conversion of pollutants into less harmful substances. It also possesses inherent. The present work concentrates on the preparation of MoS₂/BN based composite for water treatment. This undergoes various characterization studies involving-Ray Diffraction (XRD) and UV-Vis Spectroscopy analysis. This newly synthesized material could be utilized for water treatment applications.

Keywords: - field size, gradient index, brain metastasis.

INTRODUCTION

Water is an indispensable resource for life, and its sustainable management is crucial for the well-being of both humans and the environment. However, the increasing demand for clean water coupled with the escalating contamination of water sources due to industrial activities, agricultural runoff, and urbanization poses significant challenges to global water security. Consequently, there is an urgent need for efficient and eco-friendly water treatment technologies to mitigate water pollution and ensure access to safe drinking water.

Nanomaterials have emerged as promising candidates for addressing water treatment challenges owing to their unique physicochemical properties and high surface area-to-volume ratio. Among various nanomaterials, transition metal dichalcogenides (TMDs) such as molybdenum disulfide (MoS_2) and hexagonal boron nitride (h-BN) have garnered considerable attention due to their exceptional chemical stability, mechanical robustness, and biocompatibility[1]. By harnessing the synergistic properties of MoS_2 and h-BN, composite materials can be engineered with enhanced performance for water treatment applications. Molybdenum disulfide (MoS_2), a layered material composed of molybdenum atoms sandwiched between sulfur atoms, exhibits remarkable catalytic activity, adsorption capacity, and photocatalytic properties[2]. On the other hand, hexagonal boron nitride (h-BN), which shares a similar layered structure with graphene, possesses excellent thermal conductivity, chemical inertness, and hydrophobicity. By integrating MoS_2 and h-BN into a composite structure, it is possible to harness

their complementary properties to develop advanced materials for water treatment[3].

The synthesis of MoS_2 -BN composite materials involves various methods, including chemical vapor deposition (CVD), hydrothermal synthesis, and mechanical exfoliation[4]. Each synthesis route offers unique advantages in terms of scalability, cost-effectiveness, and control over material properties. For instance, CVD enables the large-scale production of high-quality MoS_2 -BN composites with precise control over composition and morphology. Hydrothermal synthesis, on the other hand, provides a facile and environmentally friendly route for the synthesis of MoS_2 -BN composites under mild reaction conditions.

The application of MoS_2 -BN composites in water treatment encompasses various processes, including adsorption, photocatalysis, and membrane filtration. The high surface area, tunable surface chemistry, and photocatalytic activity of MoS_2 -BN composites make them effective adsorbents for the removal of organic pollutants, heavy metals, and emerging contaminants from water sources. Furthermore, the integration of MoS_2 -BN composites into membranes can enhance the separation efficiency and selectivity for water purification applications[5].

In this context, this research paper aims to provide a comprehensive overview of the synthesis, characterization, and applications of molybdenum disulfide-boron nitride (MoS_2 -BN) composite materials for water treatment. By elucidating the synergistic effects between MoS_2 and BN, as well as their potential applications in water purification, this study seeks to contribute to the development of advanced materials for sustainable water

management. Overall, the integration of MoS₂ and BN into composite materials holds great promise for addressing the complex challenges associated with water treatment, paving the way for the development of next-generation technologies for clean water production and environmental remediation.

MATERIALS AND METHODS

All the materials utilized are purchased from Sigma Aldrich, USA, (AR Grade): Boron Nitride, (Molecular weight: 24.82g/mol, 99% purity AR grade), Molybdenum disulfide (MoS₂) Molecular weight: 160.07g/mol)(Density: 5.06g/cm³), Deionized water, DMF (Dimethyl Formamide) (Molecular weight: 73.10g/mol, 99% purity).

Exfoliation of BNNS using DMF

The Liquid phase exfoliation method was used for the preparation of Boron Nitride nanosheets. In this 3gm of Boron Nitride powder was dissolved in 200ml DMF (N, N-dimethylformamide) and undergoes constant stirring for about 30mins to achieve uniform dispersion by using magnetic stirrer. The dispersion was further exposed to ultrasonication process using a probe sonicator to for about 1 hour to create exfoliated nanosheets.

The supernatant solution was then agitated at 3000 rpm to get rid of any remaining unexfoliated particles. The particles are washed with deionized water after filtering and are then oven dried for about 24hours at 80°C in hot air oven.

Exfoliation of Molybdenum disulphide(MoS₂)

Liquid phase exfoliation method was used of the preparation of MoS₂ from bulk MoS₂. 2 gm of MoS₂

is mixed with 100 ml of deionized water and undergoes constant stirring for 20 minutes using magnetic stirrer for uniform dispersion. The dispersion was further exposed to ultrasonic probe sonicator for 1 hr to create exfoliated nanosheets. The supernatant solution was then agitated to 3000 rpm to get rid of any remains unexfoliated particles. The particles are washed with deionized water after filtration the sample is oven dried about 24 hrs at 80°C in hot air oven.

Preparation of Molybdenum disulfide/ BN hybrid composite

The dried substance is ground into Powder and now 50ml of DMF is added to 0.24 gm and 0.18gm of BN and stirred for 15mins. Then 0.2gm of Molybdenum disulfide (MoS₂) was added to both mixtures and stirred for 1hour using magnetic stirrer. Both the mixtures are then sonicated for 30mins. And then they are again stirred for 1hour and centrifuged. And finally, they are dried for 24hrs in hot air oven at 100°C.

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RESULTS AND DISCUSSION

XRD analysis is conducted to characterize the structural properties of materials, providing valuable insights into their crystalline structure, phase composition, and orientation. Figure 3.1(a) and 3.2(b) illustrates the XRD patterns of MOBN1 and MOBN2 respectively. The distinctive diffraction peaks corresponding to the (002), (100), (103), (105), and (110) planes observed at 2θ angles of 14°, 33°, 40°, 50°, and 59° respectively, align with the hexagonal phase of MoS₂ as per JCPDS card no: 37-1492, confirming its crystalline structure[6]. The most prominent peak in h-BN's

XRD pattern is typically around 26.02° (2theta) and corresponds to the (002) crystal plane[7]. This peak signifies the stacking of boron and nitrogen atoms in the out-of-plane direction. MOB N1 exhibits characteristic peaks at 14.40° , 26.54° , 32.48° , 35.87° , 39.56° , 43.95° , 49.59° , 58.22° , 60.34° , and 75.89° respectively(Fig 3.1(a)). In figure 1(b), MOB N2 exhibits characteristic peaks at 14.54° , 26.84° , 32.76° , 36.03° , 39.56° , 43.95° , 49.73° , 58.36° , 60.48° , and 72.92° respectively. The peak at 14.54° , corresponds to the (002) plane of MoS₂, indicating the interlayer spacing between the MoS₂ layers. These characteristic peaks confirm the presence of both molybdenum disulfide and boron nitride phases in the composite material. Additionally, the intensity and width of these peaks provide insights into the degree of crystallinity, grain size, and structural defects within the composite. The intensity of the peak at 26.84° corresponding to exfoliated BN is considered to be very weak in this composite material due to the incorporation of MoS₂ into the BN matrix thus inducing hybridization effects, modifying the electronic structure and vibrational properties of BN. This can lead to shifts or broadening of BN peaks, resulting in reduced peak intensity.

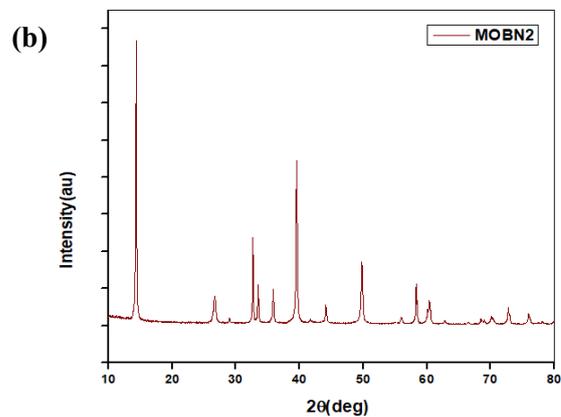
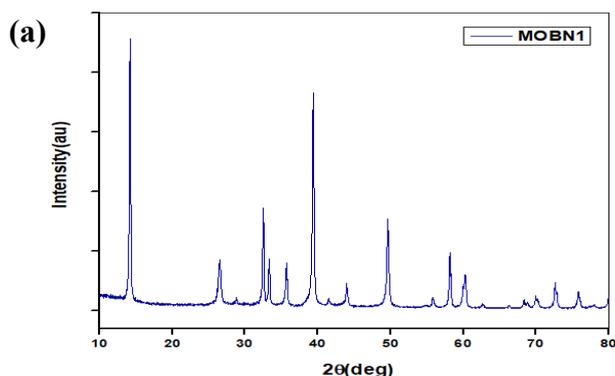


Figure 3.1: XRD analysis of (a) MOB N1 and (b) MOB N2

UV-visible analysis is a spectroscopic technique used to study the absorption, transmission, and reflection of ultraviolet and visible light by a sample. This method provides valuable information about the electronic structure, optical properties, and chemical composition of materials. Figure 3.2(a) and(b) illustrate the UV-Visible analysis graph of MOB N1 and MOB N2. MOB N1 shows an adsorption peak at 223.68nm and the corresponding bandgap energy of MOB N1 is calculated using the equation, Energy(eV) = $1240/\lambda_{\text{onset}}$ (nm), where λ_{onset} is the wavelength. MOB N1 indicates that the λ_{onset} value is 376nm and the corresponding energy is 3.29 eV. This arises due to the electronic transitions involving the energy levels of the constituent components, molybdenum disulfide (MoS₂) and boron nitride (BN). These transitions could involve the excitation of electrons from the valence band to the conduction band or from one electronic state to another within the band structure of the material. The adsorption peak of MOB N2 is at 227.72nm and the corresponding energy is 3.08eV respectively.

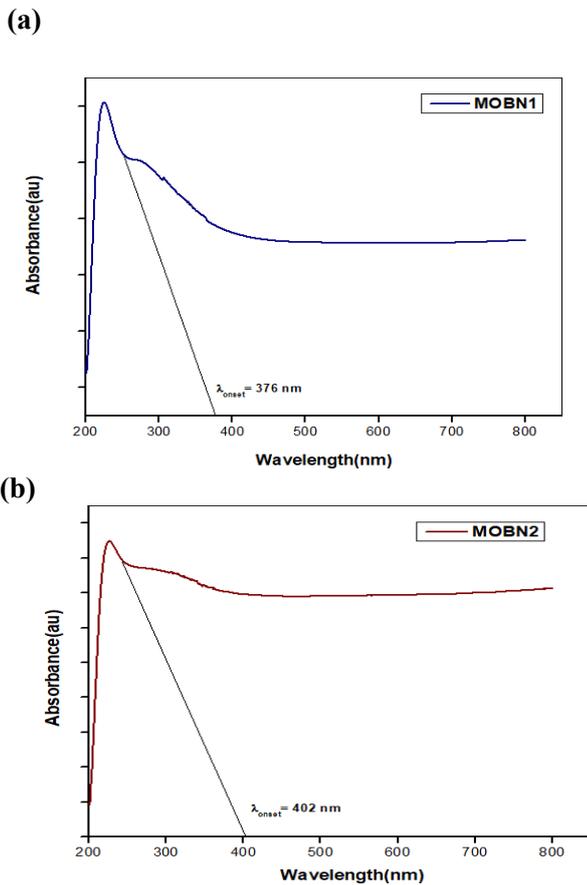


Figure 3.2: UV-Visible analysis of (a)MOBN1 and (b)MOBN2

CONCLUSIONS

The current study concentrates on the fabrication of a hybrid composite comprising Molybdenum Disulfide and Boron Nitride (MO-BN). This process entails the synthesis and exfoliation of Boron Nitride and Molybdenum Disulfide followed by the synthesis of MO-BN composites. The XRD analysis reveals the crystallinity of Molybdenum disulfide (MoS₂) and Boron Nitride (BN) within the composite, along with any potential interfacial interactions between these components. The incorporation of MoS₂ into the BN matrix induces hybridization effects that alter the electronic and vibrational properties of BN, leading to changes in the XRD peaks' intensity and profile. This

phenomenon highlights the complex interplay between different components within composite materials. FTIR spectrum of MOBN1 and MOBN2 reveals valuable information about the molecular structure and bonding characteristics of the Molybdenum disulfide-Boron Nitride composite. The onset degradation temperature of MOBN1 and MOBN2 is 124.53^oC and 146.18^oC. MOBN2 indicates a higher thermal stability compared to MOBN1. The absorption peaks observed at 223.68 nm for MOBN1 and 227.72 nm for MOBN2 correspond to electronic transitions within the composite materials. The calculated bandgap energies of 3.29 eV for MOBN1 and 3.08 eV for MOBN2 further characterize these materials' electronic structure. This recently devised material introduces a groundbreaking composite with promising practical uses. Combinations of Molybdenum disulfide and Boron Nitride provide adaptability and can be amalgamated with polymers to fabricate composite substances, broadening their applicability across different sectors of water purification. This inventive strategy amplifies the material's prospects for real-world implementation, particularly in domains requiring water-related solutions.

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