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ISOBUTYL ALCOHOL AS A SURFACE MODIFIER FOR BORON NITRIDE NANOSHEETS: SYNTHESIS AND ANALYSIS

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ABSTRACT

Addressing the escalating energy demands necessitates the development of sustainable and eco-friendly energy storage solutions, prompting exploration into novel materials. Two-dimensional (2D) materials have garnered significant interest due to their exceptional properties in recent years. Boron nitride (BN) stands out among these materials, boasting attributes such as high thermal and chemical stability, expansive surface area, wide bandgap, and advantageous mechanical and thermal characteristics. With a structure akin to graphene, hexagonal boron nitride (h-BN) has become a focal point of extensive research. Particularly, h-BN shows immense promise, with potential surface modifications poised to drive advancements in energy technologies. Various techniques are employed to tailor BN and augment its properties. This study predominantly revolves around the exfoliation of bulk boron nitride into boron nitride nanosheets through ultrasonication. Surface modification of BNNS is achieved using modifying it with isobutyl alcohol. A comprehensive characterization of the samples is done using X-ray powder diffraction (XRD), Raman spectroscopy, and Fourier-transform infrared (FTIR) spectroscopy. The utilization of isobutyl alcohol for modifying and exfoliating h-BN represents a promising avenue for the development of advanced composites with superior electrical and chemical properties, particularly for energy-related applications.

Keywords: Exfoliation, Hexagonal Boron nitride, Isobutyl alcohol, Surface functionalization

INTRODUCTION

The exhaustion of fossil fuels and the climate crisis that hangs over humanity's heads are severe challenges. Supporting the increasing demand for energy consumption is creating a demand for sustainable and affordable energy supply and storage. To address issues on global warming and the upcoming energy crisis, access to clean and renewable energy materials, and technologies is becoming a target. Solar and wind energy, as potential renewable power sources, are interrupted simply because of a lack of resources and unpredictable weather[1]. Supercapacitors, batteries, and other energy sources play a pivotal role in our day-to-day lives. The recent development of research involving two-dimensional (2D) materials, like graphene, hexagonal Boron nitride, and many others, is partly due to the significant opportunities they provide for various technological applications[2]. These materials have a great future not only in electronic devices of various types but also in sensors and catalysts. They also show significant potential as energy conversion and storage devices. They exhibit remarkable electrochemical and thermal properties and are rapidly being explored to develop new materials with enhanced features paving their usage in newer technologies.

Hexagonal boron nitride is a widely used 2D material for various energy applications due to its unique characteristic features[3]. Specifically, its excellent thermal stability, chemical resistance, and high electrical insulation ratio make it useful for energy storage and conversion. Nevertheless, as a material, h-BN possesses some limitations that affect its use in the research sector. For instance, h-BN has low conductivity when compared to alternatives like graphene. This makes it less efficient for some energy devices that heavily rely on high electricity usage. Moreover, large-scale production of high-quality h-BN is still considered a high task, which slows down the practical usage of h-BN in many applications. To address these limitations, researchers are exploring several strategies. One approach involves the synthesis of h-BN with controlled defects or doping to enhance its electrical conductivity while preserving its desirable properties. Furthermore, advancements in synthesis techniques, such as chemical vapor deposition (CVD) and exfoliation methods, are being pursued to produce high-quality h-BN films with improved scalability and uniformity. In addition to enhancing its electrical properties, efforts are underway to tailor the surface chemistry of h-BN to optimize its performance in specific energy applications[4]. Functionalization techniques, including chemical modification and surface coating, can tailor the surface properties of h-BN to improve its compatibility with electrolytes or enhance its catalytic activity in energy conversion reactions. Moreover, advancements in characterizing and understanding the fundamental properties of h-BN at the nanoscale are crucial for guiding the design of next-generation energy devices[5]. Isobutyl alcohol (IBA), ($(CH_3)_2CHCH_2OH$), also known as 2-methyl-1-propanol, is a colorless liquid with a distinctive odor

Isobutyl alcohol is commonly used as a solvent in various industrial applications due to its excellent solubility in both polar and non-polar substances. One of the key properties of isobutyl alcohol is its relatively low boiling point, which makes it easy to evaporate and remove from reaction mixtures or solvent systems. This characteristic is advantageous in processes where the residual solvent needs to be minimized. In the realm of energy devices, isobutyl alcohol finds application in various capacities. One notable usage is in the fabrication of electrolytes for energy storage systems, particularly in redox flow batteries (RFBs). Isobutyl alcohol can serve as a solvent for dissolving electrolyte salts, enabling the creation of electrolyte solutions with tailored properties such as conductivity and viscosity. It can also serve as a precursor or solvent in the preparation of electrode materials for batteries or fuel cells. By dissolving or reacting with appropriate precursors, isobutyl alcohol can help facilitate the formation of desired materials with controlled morphology and composition, ultimately influencing the performance of energy devices. This research work concentrates on the functionalization of boron nitride using IBA. During the functionalization process, the hydroxyl group (-OH) of isobutyl alcohol can undergo a chemical reaction with certain surface sites on h-BN. This reaction can lead to the formation of covalent bonds between the isobutyl groups and the h-BN surface, resulting in the attachment of the isobutyl functional groups onto the h-BN surface. The introduction of isobutyl functional groups onto the surface of h-BN can impart new properties and functionalities to the material. It could alter the surface chemistry of h-BN, making it more compatible with certain solvents or polymers. Additionally, the presence of isobutyl groups can modify the surface energy of h-BN, influencing its interactions with other materials in composite systems or enhancing its dispersibility in solution.

In this study, bulk boron nitride (BN) is subjected to an exfoliation process followed by ultrasonication to produce exfoliated Boron nitride. This is then surface-modified using isobutyl alcohol, an organic compound primarily employed as a solvent. This method of functionalization, being introduced for the first time, aims to enhance the properties of BNNS. The research presents a comparative analysis between the original bulk BN material and the newly functionalized sample. Various characterization techniques are employed to analyze the prepared samples. The surface-functionalized boron nitride is subsequently incorporated as a nanofiller into different polymers to augment their performance potential across various applications. The exceptional properties of boron nitride and its composites are envisioned to advance their utilization in energy-related fields.

EXPERIMENTAL

Isobutyl alcohol (with a molecular weight of 74.12 g/mol) and DMF are supplied by specialized professionals at Merck in India. BN powder (with a molecular weight of 24.82 g/mol, particle size of approximately 1 µm, and a density of 2.29 g/ml at

25°C) is procured from Sigma Aldrich in the United States, and all the chemicals are of analytical grade.

To exfoliate Boron nitride, the appropriate amount of BN is heated to 80°C to remove excess moisture. The heated BN powder is then thoroughly mixed with DMF and stirred continuously for 25 minutes to ensure even dispersion. Subsequently, the dispersion undergoes ultrasonication for one hour using a probe sonicator to achieve exfoliated BN. The resulting mixture is vigorously agitated at 2000 rpm to eliminate any remaining unexfoliated particles. After filtration, the particles are washed with distilled water and dried in an oven at 80°C for a day before being ground into powder and sealed in zip-lock covers. For the surface modification of BNNS using isobutyl alcohol (IBA), a solution containing 100 ml of water and a 3 M concentration of IBA is prepared and stirred for 30 minutes. The exfoliated BN is then mixed with this 3 M concentration of IBA and thoroughly stirred for three hours. The BNNS dispersed in IBA (BNIB) are subsequently oven-dried at 80°C for approximately 72 hours. Following drying, the sample is reheated at 400°C in a muffle furnace to ensure successful attachment of the IBA to the exfoliated, with an increase in furnace temperature facilitating this process.

RESULTS AND DISCUSSION

All samples underwent characterization using various analytical techniques. X-ray diffraction (XRD) analysis was conducted using the X-PERT-PRO X-ray Diffractometer with CuKα radiation (λ=1.5218 Å). Fourier Transform Infrared Spectroscopy (FTIR) was performed using the FTIR spectrometer Braker Alpha. Raman spectroscopy analysis was carried out using the HR 800 micro-Raman instrument from HORIBA Jobin Yovon, France.

By analysing the diffraction patterns of materials, X-ray diffraction (XRD) technique is a potent technique used to ascertain the crystal structure and purity of materials. A clear peak at 26.620, which corresponds to the (002) hkl plane of exfoliated boron nitride nanosheets (BNNS), is seen in Figure 1(a). In the XRD study of boron nitride nanosheets, additional peaks were seen at crystallographic planes like (100), (101), (102), (004), and (110), which indicate the existence of crystal orientations and lattice planes. Following XRD analysis of exfoliated BN, isobutyl alcohol is used to modify the surface of the exfoliated BN. The diffraction spectrum of BNIB shows the introduction of newer peaks, which validates the surface functionalization. The diffraction peaks are obtained at 14.82°, 26.40°, 30.79°, 41.69°, 54.69°, 63.45°, and 75.75° are shown in Figure 1(b) for the BNIB sample. This indicates a minor variation of 0.22° for the (002) hkl plane of BNNS.

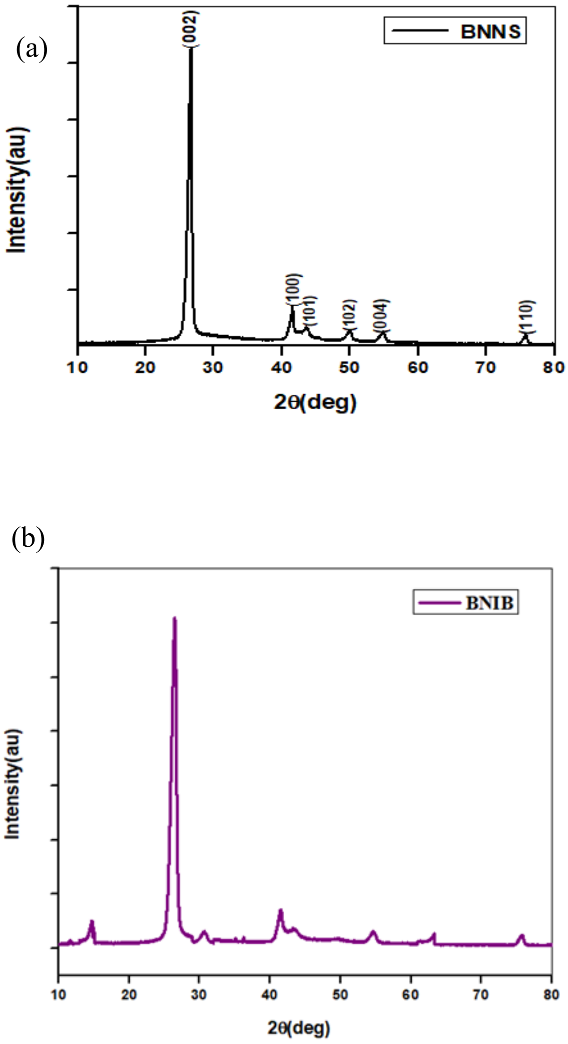


Figure 1: XRD interpretation of (a) BNNS and (b) BNIB

The FTIR spectral analysis of various materials including BNNS and BNIB was conducted over a broad range of wavelengths from 400 to 4000 cm^{-1}. In Figure 2(a), two prominent peaks are evident in the BNNS spectrum at 812.14 cm^{-1} and 1382.71 cm^{-1}, indicating successful transformation from bulk BN to BNNS through exfoliation. No other significant peaks were detected in the exfoliated BN spectrum. Surface modification of exfoliated BN using isobutyl alcohol resulted in noticeable changes in its FTIR spectrum. A peak at 3450.18cm^{-1} is observed in BNIB that corresponds to the stretching vibration of the hydroxyl group (-OH) present in the isobutyl alcohol(Fig 2(b)). This peak indicates the presence of hydroxyl groups on the surface of the functionalized boron nitride, suggesting successful functionalization with isobutyl alcohol. A highly intense V-shaped peak is also observed at 1386.50cm^{-1} in the FTIR spectrum of boron nitride functionalized with isobutyl alcohol indicating a significant chemical interaction between the boron nitride surface and the isobutyl alcohol molecules. This peak becomes more intense due to the formation of new chemical bonds or the alteration of existing bonds between the functional groups of isobutyl alcohol and the surface atoms of boron nitride.

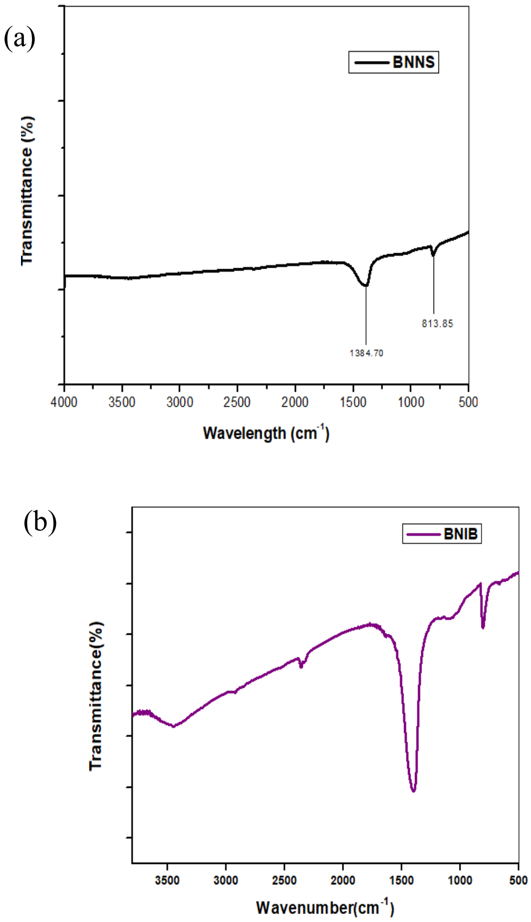
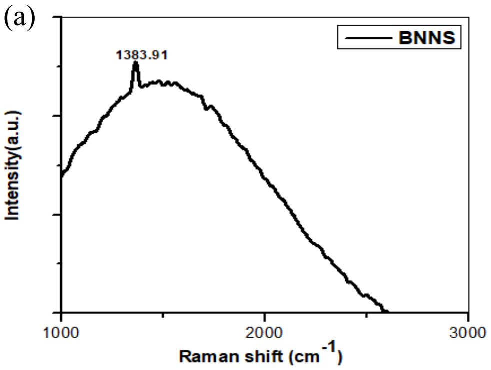


Figure 2: FTIR analysis of (a)BNNS and (b) BNIB

Raman spectroscopy is a valuable tool for understanding material composition and structure, as well as molecular interactions. The Raman spectra of BNNS and BNIB primarily show in-plane vibrational modes (E_{2g}). In Figure 3(a), the Raman spectrum of BNNS displays a peak at 1383.91 cm^{-1}, consistent with previous findings [6]. This peak corresponds to in-plane displacement vibrations caused by boron and nitrogen atoms in BNNS. Surface functionalization can lead to shifts in these peaks, either towards longer (red) or shorter (blue) wavelengths, indicating alterations in sample quality due to surface modifications. In Figure 3(b), the Raman spectrum of BNIB reveals a peak at 1391.97 cm^{-1}, with a blue shift of 7.89 cm^{-1}. This shift signifies alterations in the material's chemical structure and lattice vibrations. Specifically, in Raman spectroscopy, such shifts in peak positions reflect changes in the bonding environment or molecular interactions within the material. The blue shift observed here suggests modifications in the molecular configuration or bonding patterns of BNIB, potentially due to surface functionalization or other structural changes.

(a)



(b)

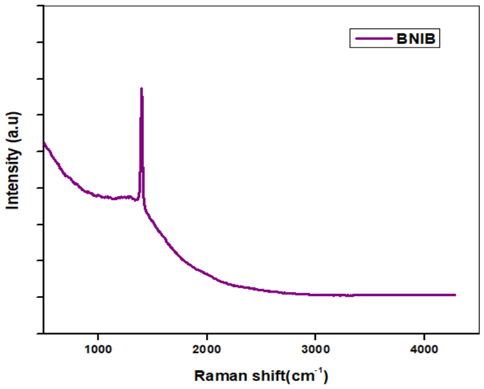


Figure 3: Raman analysis of (a)BNNS and (b) BNIB

CONCLUSION

This study focuses on synthesizing and characterizing surface-modified boron nitride nanosheets. Bulk BN undergoes exfoliation processes to produce BNNS, followed by surface functionalization using isobutyl alcohol. Various characterization techniques are employed to analyze the synthesized samples. X-ray diffraction (XRD) analysis confirms BNNS formation, with new peaks in the XRD diffraction spectrum indicating the incorporation of the OH group in BNNS. The increased peak intensity in the XRD data BNIB suggests a maintained crystalline nature of BNNS after surface modification and a thickness increase in BNNS layers. FTIR spectra show newer peaks with hydroxylation in BNIB compared to BNNS respectively. Detailed Raman spectra analysis is also conducted. This innovative material shows potential for practical use and could be combined with polymers to produce composites, broadening its applications in energy-related sectors. Utilizing isobutyl alcohol to functionalize boron nitride presents a novel material choice with diverse application possibilities.

AUTHOR CONTRIBUTIONS

All authors participated in the collaborative development of the manuscript, making active contributions throughout its creation. The final version of the draft garnered unanimous approval from all contributors. The authors also affirm that they have no competing conflicts of interest to disclose.

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