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FERRIC CHLORIDE-MEDIATED SYNTHESIS AND SURFACE MODIFICATION OF BORON NITRIDE NANOSHEETS

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ABSTRACT

Boron nitride nanosheets (BNNS) have garnered significant attention generated because of their exceptional properties, including high thermal conductivity, chemical inertness, and mechanical strength. Surface modification techniques play a crucial role in tailoring the properties of BNNS for various applications. In this study, we introduce an innovative method for surface modification of BNNS utilizing Ferric chloride hexahydrate ($FeCl_3 \cdot 6H_2O$). The modification process involves the reaction occurring chemically between ferric chloride and BNNS, leading to the formation of a stable coating or functional groups on the BNNS surface. The modified BNNS exhibit improved dispersion in solvents and enhanced compatibility with polymers, facilitating their incorporation into composite materials. Moreover, the modified BNNS demonstrate properties related to heat and mechanical aspects that renders them potentially suitable for various applications in thermal management, reinforcement in polymers, and electronic devices. The research offers significant understanding the surface modification of BNNS using ferric chloride, opening avenues for further exploration in advanced materials science and engineering. Various structural analysis techniques are utilized to characterize the resultant samples, comprising XRD, Raman and FTIR spectroscopy.

Keywords: *- Boron Nitride, Ferric chloride hexahydrate, Surface Modification, Water Treatment*

INTRODUCTION

h-BN, a close structural analogue to graphite, has garnered considerable focus due to its prominence remarkable attributes and versatile implementation. Its two-dimensional layered structure, composed of hexagonally arranged boron and nitrogen atoms, imparts exceptional stability in terms of heat and chemical resistance, superior mechanical strength, and excellent electrical insulation properties [1]. In the context of water purification, the surface functionalization and modification of h-BN play a crucial role in enhancing its performance as an adsorbent or membrane material for the eviction of contaminants from water supply. Functionalization refers to the deliberate introduction of specific functional groups or chemical moieties onto the surface of h-BN nanosheets, aiming to tailor their surface properties to better suit the desired application [2].

One prominent approach involves the use of suitable reagents to achieve surface functionalization of h-BN for water treatment applications. These reagents are selected based on their ability to engage with the surface of h-BN and introduce functionalities that enhance its adsorption capacity, selectivity, and stability in aqueous environments. One such reagent that has shown promise in surface modification of h-BN for water purification is ferric chloride hexahydrate ($FeCl_3.6H_2O$)[3] this compound, commonly reffered to as ferric chloride, exhibits unique charecteristics that make it particularly effective in surface modification and treatment of water contaminants. One of the key attributes of ferric chloride hexahydrate is its ability to functionalize various surfaces, including nanoparticles, nanosheets, and porous materials. When employed as a reagent for surface modification, $FeCl_3.6H_2O$ interacts with functional groups present on the materials surface, results in the introduction of new chemical moieties or surface complexes. This functionalization process can alter the surface properties of materials, such as their hydrophilicity, surface charge, and chemical reactivity, thereby enhancing their performance in specific applications [4].

It serves as a versatile reagent capable of chemically modifying the surface of h-BN nanosheets, leading to the initiation of hydrophilic functional moiety such as hydroxyl (-OH) and carboxyl (-COOH) groups. They not only enhance the dispersion capability of h-BN in water but also increase their affinity towards waterborne contaminants, thereby improving its adsorption efficiency [5]. This modification can result in improved dispersion, stability, and compatibility of BNNS with various matrices or solvents, thus facilitating their incorporation into composite materials or enhancing their performance in specific applications. Additionally, surface modification using $FeCl_3.6H_2O$ can impart catalytic activity to h-BN, enabling the degredation of organic pollutants through advanced oxidation processes, further enhancing its efficacy in water purification applications. In summary, the surface functionalization and modification of hexagonal boron nitride using suitable reagents such as ferric

chloride hexahydrate hold immense potential for water purification applications. By tailoring the surface chemistry of h-BN nanosheets, these approaches aim to improve their adsorption capacity, selectivity, and stability, contributing to the development of efficient and sustainable solutions for clean water access [6].

MATERIALS AND METHODS

The required quantity of BN was taken and heated to 80^0C to eliminate the level of moisture. After preheating, the fine particles was blended with DMF and stirred together thoroughly for 15 minutes to achieve homogeneous dispersion. Following this, the dispersion underwent ultra sonication for approximately 60 minutes to produce nanosheets. Subsequently centrifugation at 6000 rpm was done to separate any residual particles. Grains that have undergone filtration was then rinsed using deionized water and subsequently dried using oven at 80°C for a duration of one day. Once parched, the material was ground into a powder and functionalized using $FeCl_3.6H_2O$. The BN-$FeCl_3$ mixture was prepared by thoroughly mixing 100ml of deionized water with BN in ratios of 1:2. This dispersed solution was then placed in a hot oven at 80°C for 24 hrs. particles. The remaining evaporated samples was powdered and stored in

.

RESULTS AND DISCUSSION

The powder samples are subjected to X-ray diffraction (XRD) analysis to examine their phase structure and crystal purity. The XRD spectra of BNNS and FCBN are depicted in Fig 3.1(a) and 3.1(b) respectively. The characteristic peak of exfoliated BN appears at 26.63^0, corresponding to the (002) hkl planes of h-BN. Upon treatment of BNNS with Ferric chloride, additional peaks emerge. Figure 3.1(b) illustrates peaks at 33.21^0, 35.50^0, 53.95^0, 63.83^0, confirming the incorporation of Ferric chloride.

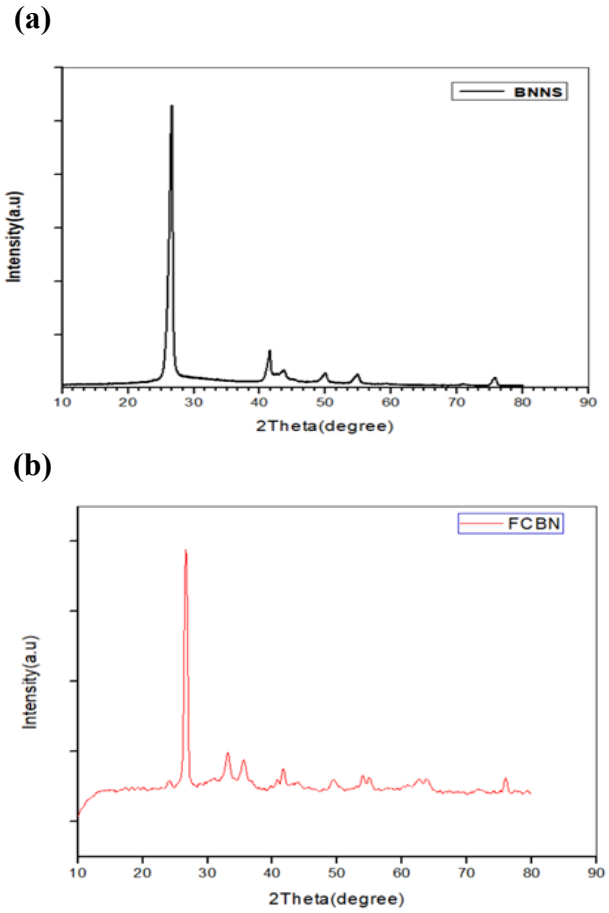

Figure 3.1: X-ray diffraction spectrum of (a) BNNS, (b) FCBN

In analyzing Raman spectrum, shifts in peaks can be identified. Depending on the quality of exfoliation, either a red or blue shift can be observed. In Figure 3.2 (a), the Raman spectrum of BNNS is depicted, showing a high intensity peak at 1367 cm^{-1}. Moderate intensity peaks are attributed to E_{2g} phonons [7]. The prepared composite exhibits a shift from BNNS due

to functionalization and surface modification. Figure 3.2(b) illustrates the Raman spectra of FCBN, showing a peak of higher intensity at 1398.1 cm^{-1} and a significant blue shift of 192.87 cm^{-1} compared to BNNS. These shifts in peaks are attributed to compressive strain in the sample and long-range interlayer interaction of ferric chloride -modified BNNS.

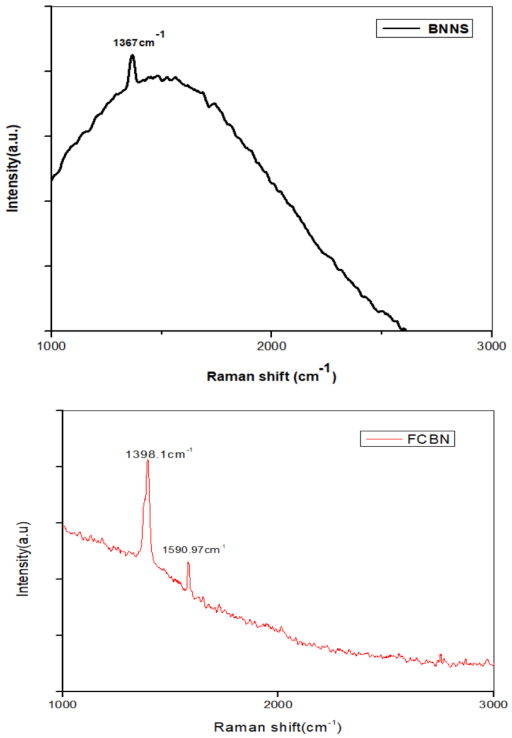

Figure 3.2 :Raman spectra of (a) BNNS, (b) FCBN

The FTIR analysis of BNNS and FCBN is conducted within the range of 400-4000 cm^{-1} and

is displayed in figures 3.3(a) and 3.3(b). The exfoliated BNNS exhibits prominent peaks at 812.59 cm^{-1} and 1381.80 cm^{-1}, indicating the exfoliation of bulk BN to form BNNS, with no further peaks observed. The FTIR spectrum of FCBN1, peaks are observed at 3178.80 cm^{-1}, 2358.47 cm^{-1}, 1395.02 cm^{-1}, 806.37 cm^{-1}. In FCBN at 806.37 cm^{-1} and 1395.02 cm^{-1} the occurrence of steak peak convey existence of BNNS, while all remaining characteristic peaks suggest the surface alteration of BNNS using Ferric chloride. Broad peaks with medium intensity at 3178.07 cm^{-1} reveal the presence of a chloride group, covalently attached to the electrophilic sites of boron in BN.. The 803.23 cm^{-1} peak signifies vibrations originating from the bonds between Fe and oxygen, whereas the 1395.02 cm^{-1} peak is indicative of the stretching motion of boron and nitrogen bonds.

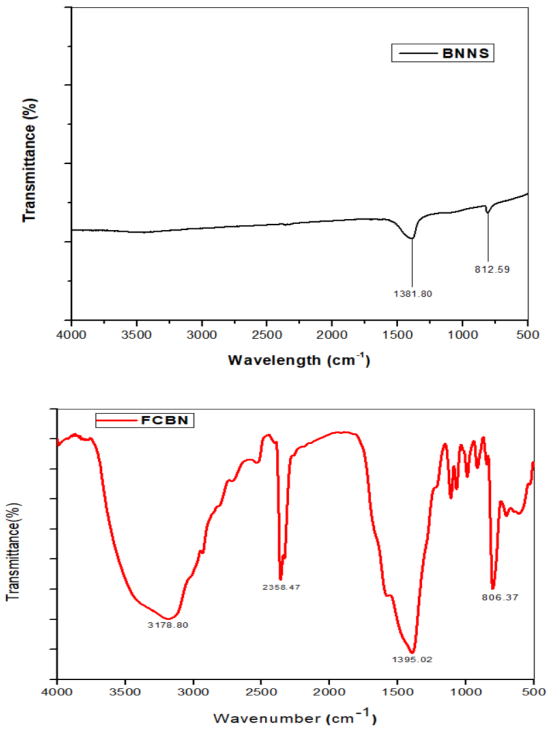

Figure 3.3 : FTIR of (a) BNNS, (b) FCBN

CONCLUSIONS

The focus of this study lies in the synthesis and characterization of surface-modified boron nitride nanosheets (BNNS). Bulk BN is subjected to exfoliation techniques to yield BNNS, which are subsequently mixed with Ferric chloride. Surface

functionalization of BNNS is achieved by the use of Ferric Chloride hexahydrate. Various characterization methods are employed to analyze the prepared samples. XRD analysis confirms the formation of BNNS, with the presence of new peaks in the diffraction spectrum indicating the incorporation of the OH group in BNNS. Higher peak intensity suggests an increase in the thickness of BNNS layers. FTIR spectra reveal the existence of the modifier cluster, Ferric chloride, having a broad crest indicating the presence of the chloride group in the samples. Raman spectra of BNNS and FCBN, demonstrate a significant blue shift relative to BNNS, with shifts of 192.87 cm^{-1} observed. This newly synthesized material is a novel material that could be utilized for water treatment applications.

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