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Investigation of Borophene Synthesized via a Scalable Approach as an Anode Material for Lithium-Ion Batteries

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Abstract: Borophene is considered as a promising anode material for lithium-ion batteries due to its high specific capacity and low diffusion barrier. However, practical applications exploring borophene as an anode material remain very limited. In this study, the anode performance of borophene synthesized via a scalable electrochemical exfoliation method, was investigated in lithium-ion batteries (LIBs). The obtained borophene sample was structurally characterized using X-ray photoelectron spectroscopy (XPS), high-resolution transmission electron microscopy (HRTEM), and atomic force microscopy (AFM). The electrochemical performance of the anode was evaluated by assembling CR2032 type coin cell. Galvanostatic charge/discharge tests showed that the initial discharge capacity of the borophene anode was 387 mAh g⁻¹ at 0.1 C, which only dropped to 371 mAh g⁻¹ after 10 cycles, exhibiting 95.8% capacity retention rate. These results indicate that borophene holds a substantial potential as an anode material for lithium-ion battery applications.

Keywords: Borophene, Electrochemical exfoliation, Li-ion batteries.

Introduction

The ever-increasing global energy demand has brought the need for high-energy-density and long-life energy storage technologies to the forefront (Tarascon et al., 2001). In this context, lithium-ion batteries remain one of the most widely used energy storage systems due to their high energy efficiency and long cycle life (Lökçü et al., 2023; Çelikkilek et al., 2022). However, the currently commercialized anode material, graphite, suffers from a low theoretical capacity, making it insufficient to meet the performance requirements of next-generation energy storage systems (Etacheri et al., 2011). Consequently, significant research efforts have been directed toward developing alternative anode materials that can provide higher capacities, faster ion diffusion and improved cycling stability (Manthiram, 2020).

Two-dimensional (2D) materials have attracted substantial attention in this regard due to their high surface area, short ion diffusion paths and tunable electronic structures (Chhowalla et al., 2013). Although various 2D materials such as graphene, phosphorene, and transition metal dichalcogenides (TMDs) have been extensively investigated, many of them still suffer from drawbacks such as low chemical stability or limited capacity (Can et al., 2024; Voiry et al., 2015). At this point, borophene emerged as a promising candidate for diverse energy-related applications owing to its structural diversity and theoretically high lithium storage capacity (Can et al., 2024; Adekoya et al., 2024). Computational studies have revealed that borophene sheets can easily adsorb lithium ions, exhibit low diffusion barriers and achieve theoretical capacities exceeding 1000 mAh g⁻¹ in certain phases (Zhang et al., 2016). These remarkable properties position borophene among the most promising candidates for fast-charging and high-energy-density anode materials (Ashraf et al., 2023). Recently, electrochemical exfoliation has emerged as a promising alternative approach for borophene fabrication (Sielicki et al., 2022). This method relies on the electrochemical delamination of layered boron precursors under suitable electrolyte conditions,

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offering an environmentally friendly, low-temperature and scalable route for borophene production. Nevertheless, several challenges remain for the practical implementation of borophene. Freestanding borophene sheets are thermodynamically unstable and readily oxidize upon exposure to air (Arnold et al., 2020). In addition, structural degradation can occur during repeated electrochemical cycling, leading to limited cycle life. To overcome these limitations, heterostructures composed of borophene and other 2D materials, such as graphene, have been reported to enhance mechanical stability and improve electron/ion transport (Kaçar et al., 2023; Yu et al., 2020). As a result, borophene-based composites hold great promise for developing next-generation anode systems that combine high capacity with excellent cycling durability.

In this study, borophene powder obtained via an electrochemical exfoliation process were investigated as an anode material for lithium-ion batteries. The structural and morphological properties of the synthesized product were characterized using AFM, HRTEM and XPS analyses. Electrochemical charge–discharge measurements were performed to study the electrochemical lithium storage properties of borophene.

Materials & Methods

The electrochemical exfoliation method of borophene was described in a recent study (Can et al., 2024). Briefly, 375 mg of crystalline boron, 125 mg of multi-walled carbon nanotubes (MWCNTs) and 50 mg of polymethyl methacrylate (PMMA) dissolved in acetone were mixed to obtain a homogeneous blend. The mixture was further homogenized in isopropyl alcohol (IPA) using bath sonication and subsequently dried overnight at 80 °C. The dried powder was then compacted into circular pellets under a pressure of 500 bar using a manual hydraulic press to prepare electrodes suitable for electrochemical exfoliation.

The exfoliation process was carried out in a 1:1 (v:v) mixture of 1 M sodium sulfate (Na_2SO_4) and glycerol under a constant voltage of 30 V. During the exfoliation, MWCNTs served as conductive pathways, facilitating electron transfer. After exfoliation, the MWCNTs were removed through a two-step purification process. In the first step, the exfoliated borophene sheets were dispersed in the aqueous phase of a toluene/water biphasic system, where sonication enabled the accumulation of MWCNTs at the interface. The remaining nanotubes were further eliminated by filtration through a cellulose membrane with an 8 μm pore size. The purified borophene nanosheets were redispersed in a 1:1 (v:v) H_2O /IPA mixture and centrifuged at 4500 rpm for 20 min. Finally, the borophene powder was obtained by freeze-drying at -37 °C and 0.18 bar for 24 h.

For anode preparation, the borophene powder, Super P carbon black and PVDF binder (in a weight ratio of 75:15:10) were mixed in N-methyl-2-pyrrolidone (NMP) using a ball mill to form a homogeneous slurry. The resulting mixture was coated onto copper foil and dried under vacuum at 80 °C for 12 h. Electrochemical performance tests were conducted using CR2032-type coin cells. The cells were assembled in an argon-filled glove box where H_2O and O_2 levels were maintained below 0.1 ppm. Lithium metal served as both the counter and reference electrode, while a polypropylene (Celgard 2400) membrane was used as the separator. The electrolyte consisted of 1 M LiPF_6 dissolved in a 1:1 (v:v) mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC).

AFM measurements were obtained in tapping mode using a Hitachi 5100N microscope. HRTEM was conducted on an FEI TALOS F200S TEM instrument. XPS analyses were performed using a SPECS FlexMod spectrometer equipped with an Al-K α radiation source (1486.71 eV). Galvanostatic charge–discharge tests were performed using a Gamry Reference 3000 Potentiostat/Galvanostat/ZRA within a potential range of 0.1–3.00 V (vs. Li^+/Li) at a current rate of 0.1 C.

Results and Discussion

AFM analyses were conducted to investigate the surface topography and layer thicknesses of the borophene sheets (Figure 1). The measurements reveal that the layer thicknesses vary between 2.2 and 6.2 nm. This broad distribution indicates that the borophene exhibits structures ranging from few-layered to multilayered sheets, reflecting variability in exfoliation efficiency and surface area among the sheets. The HRTEM observations of the electrochemically exfoliated borophene reveal that the material exhibits a crystalline and multilayered structure (Figure 2). Distinct crystalline domains can be clearly observed and the interlayer spacing is measured to be approximately 4.7 Å (Figure 2b), which matches with the (021) plane of β -rhombohedral borophene. This value is consistent with the interlayer distances reported for borophene in the literature, confirming the successful formation of few-layer borophene structures (Zielinkiewicz et al., 2023).

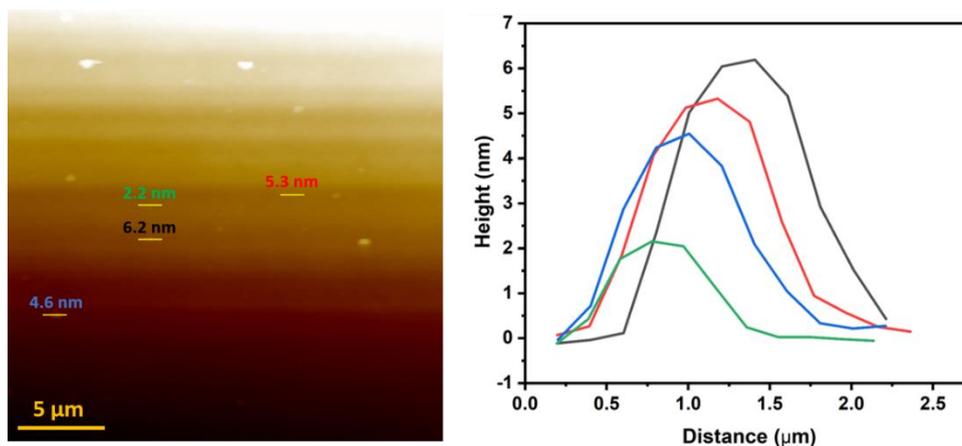


Figure 1. AFM image and the corresponding height profiles of some borophene sheets dispersed on Si substrate.

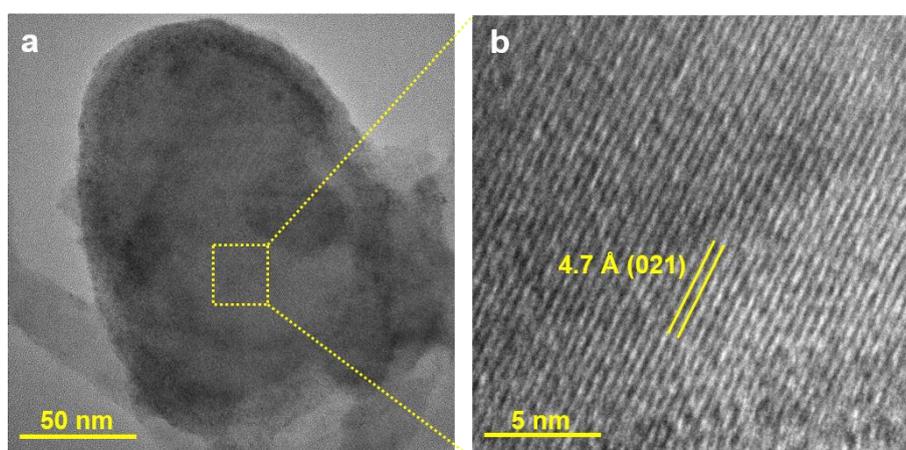


Figure 2. HRTEM images of electrochemically exfoliated borophene sheet.

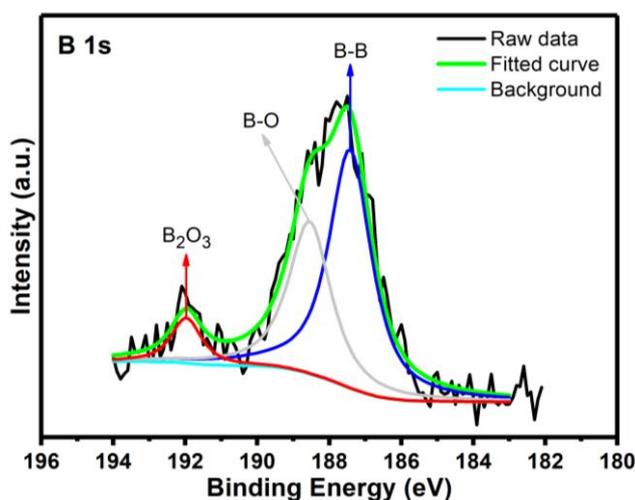


Figure 3. B 1s XPS spectrum of electrochemically exfoliated borophene sheets.

The B 1s XPS spectrum provides detailed information on the chemical composition and oxidation states of the borophene sheets (Figure 3). The spectrum consists of three main peaks located at 187.4 eV (B–B), 188.6 eV (B–O) and 192.0 eV (B_2O_3). The presence of B–O bonds indicates surface oxidation of borophene upon air exposure, whereas the B_2O_3 component can be attributed to electrochemical oxidation reactions occurring during the exfoliation process. These findings confirm that the borophene contains predominantly B–B bonding along with surface oxidation species, which is consistent with previous reports in the literature (Can et. al., 2024). The lithium storage performance of the borophene electrodes was evaluated through galvanostatic charge–discharge cycles at a current rate of 0.1 C (Figure 4). The first three cycles were applied as an activation process to ensure structural

stabilization of the electrode and complete interaction with the electrolyte. Following the activation cycles, the initial discharge capacity was measured as 387 mAh g^{-1} , indicating the effective lithium storage capability of the borophene-based anode. After 10 cycles, the capacity remained at 371 mAh g^{-1} , corresponding to approximately 95.8% capacity retention, demonstrating excellent cycling stability of the material. Moreover, the coulombic efficiency remained consistently high throughout the cycles, reaching 97.3% by the 10th cycle.

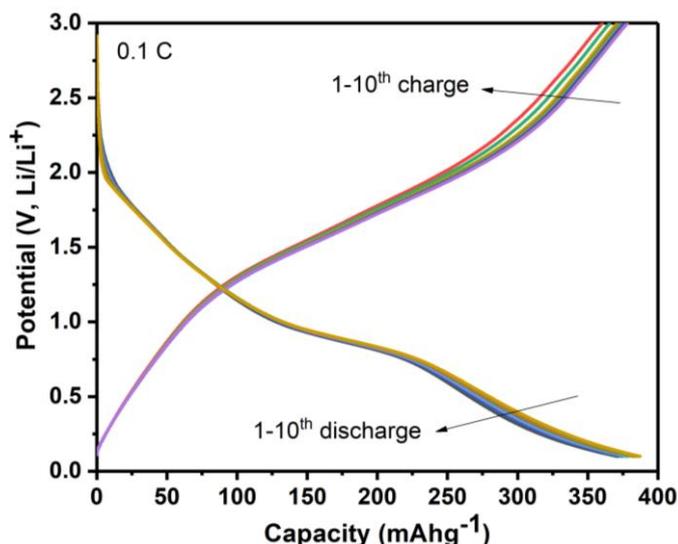


Figure 4. Galvanostatic charge–discharge performance of borophene electrode at 0.1 C.

This result indicates that the electrode structure remains stable during repeated charge–discharge processes and that the reversibility of lithium ion insertion/extraction is well maintained. These findings suggest that borophene anodes synthesized via a scalable method represent promising candidates for lithium-ion batteries, offering high cycling stability, good capacity retention and excellent coulombic efficiency.

Conclusion

In summary, electrochemically exfoliated borophene sheets were successfully synthesized and comprehensively characterized using AFM, HRTEM and XPS analyses. The results confirmed that the material exhibits a crystalline, multilayered structure with a partially oxidized surface. When employed as an anode material LIBs, the borophene electrodes demonstrated a high initial discharge capacity of 387 mAh g^{-1} and excellent cycling stability, retaining 95.8% of the capacity after ten cycles. The coulombic efficiency remained consistently high, reaching 97.3% at the 10th cycle, indicating good reversibility of lithium ion insertion/extraction and structural stability of the electrodes. These findings highlight the potential of borophene anodes synthesized via a scalable, electrochemical exfoliation approach as promising candidates for next-generation lithium-ion batteries, combining high capacity, robust cycling performance and excellent coulombic efficiency.

Scientific Ethics Declaration

* The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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