

Highly efficient & stable Bi & Sb anodes using lithium borohydride as solid electrolyte in Li-ion batteries

(Electronic Supplementary Information)

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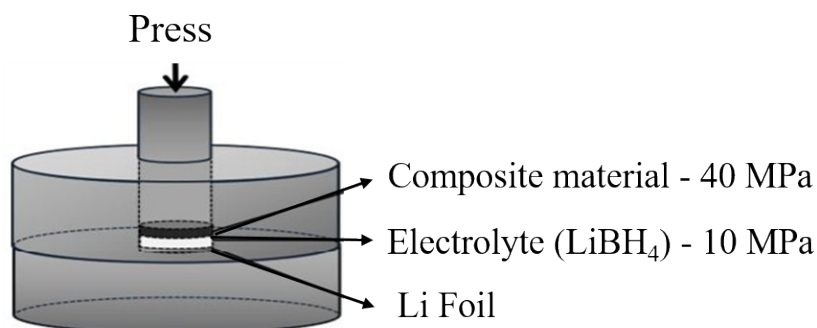
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Experimental Details

Two coin cells constituting of Bi-LiBH₄-AB|LiBH₄|Li & Sb-LiBH₄-AB|LiBH₄|Li have been fabricated to perform the electrochemical tests. The commercially available bulk Bi (Alfa aesar 99.999%), and Sb (Rare Metallic Co. Ltd. 99.9%) were used as received, whereas as-purchased LiBH₄ (Sigma Aldrich, 95%) and acetylene black (AB) were dried under vacuum at 200°C for 24 hr before using these for the preparation of negative electrode material. LiBH₄ and AB were used to enhance the ionic and electrical conductivity of the anode materials. The negative electrodes were prepared by ball milling of Bi/Sb, LiBH₄ and conductive carbon (acetylene black AB) in 40:30:30 weight ratio for 2hrs with one hr milling and 30 min rest pattern. The ball milling was carried out in a hardened stainless steel ball of 7 mm in diameter. The milling of 200 mg anode material was performed with 10 SS balls at 370 rpm using Fritsch P7. To measure the electrochemical performance of Bi/Sb anode material, a coin cell was fabricated using a three-layer pellet. Li-foil on SS plate was used as the first layer, working as cathode. The second layer was prepared by spreading the solid electrolyte LiBH₄ (80 mg) on the Li-foil and applying a pressure of 10 MPa for 5 min. Then the prepared anode composite powder (10 mg) was spread on the two-layered pellet and pressed with 40 MPa pressure for 5 min. Then, this 3-layer pellet was placed in a coin cell and sealed with Perfluoroalkoxy (PFA) gasket. A charge-discharge analyzer (HJ1001SD8, Hokuto Denko Co.) was used to observe the electrochemical performance

of Bi/Sb vs. *Li* – metal, by Galvanostatic charge-discharge measurements at an optimized rate of 0.1C. To obtain the fast Li^+ conduction from LiBH_4 , all electrochemical measurements in this study were conducted at 120°C by using a silicon oil bath as the heating source. The potential window for charging-discharging cycles was optimized by cyclic voltammetry (CV), performed on a Bio logic SAS (SP-150) system. The galvanostatic charging/discharging profile was recorded using Hokuto Denko Charge/Discharge Unit (HJ-SD8). The electrochemical reaction mechanism was identified using powder X-ray diffraction (XRD) performed at different stages of electrochemical charging/discharging.



Schematic diagram of the coin cell fabrication

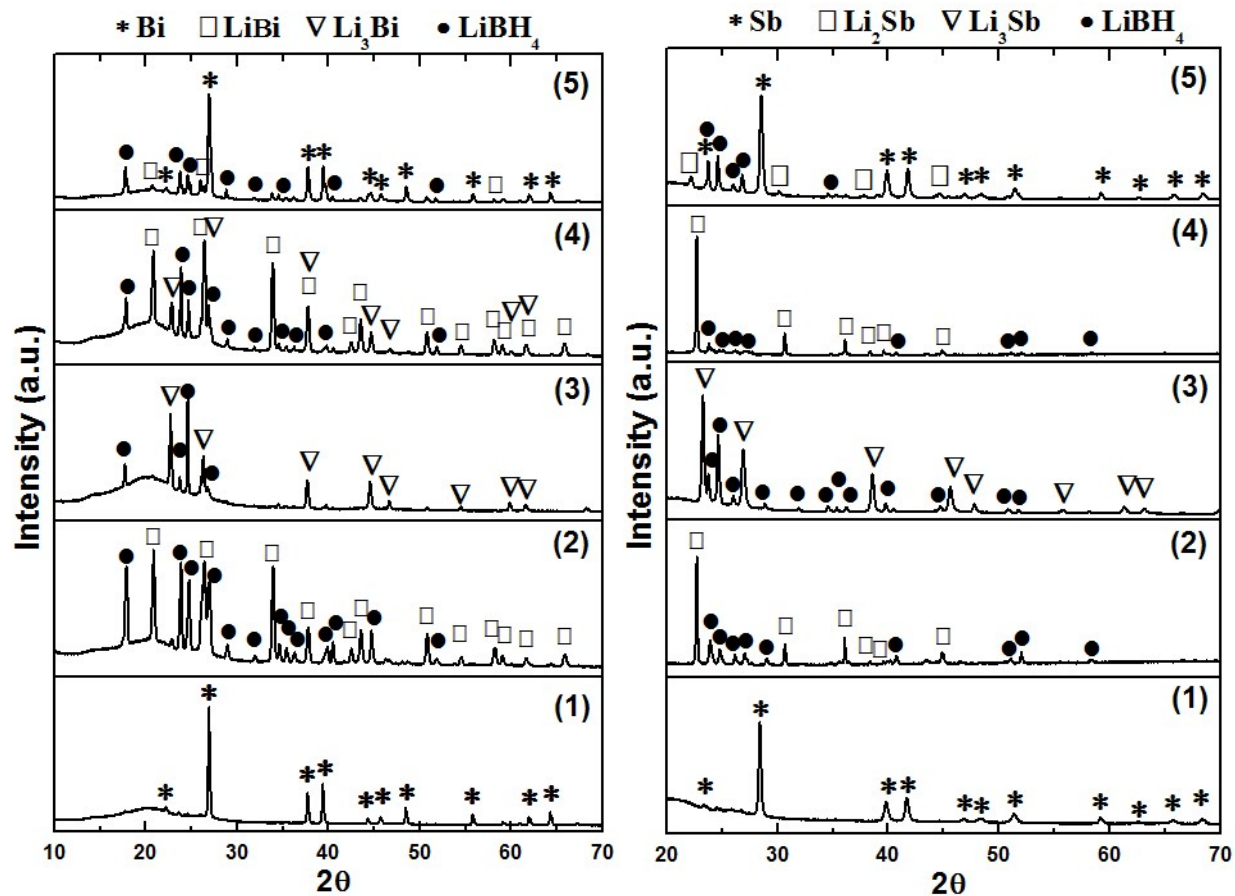
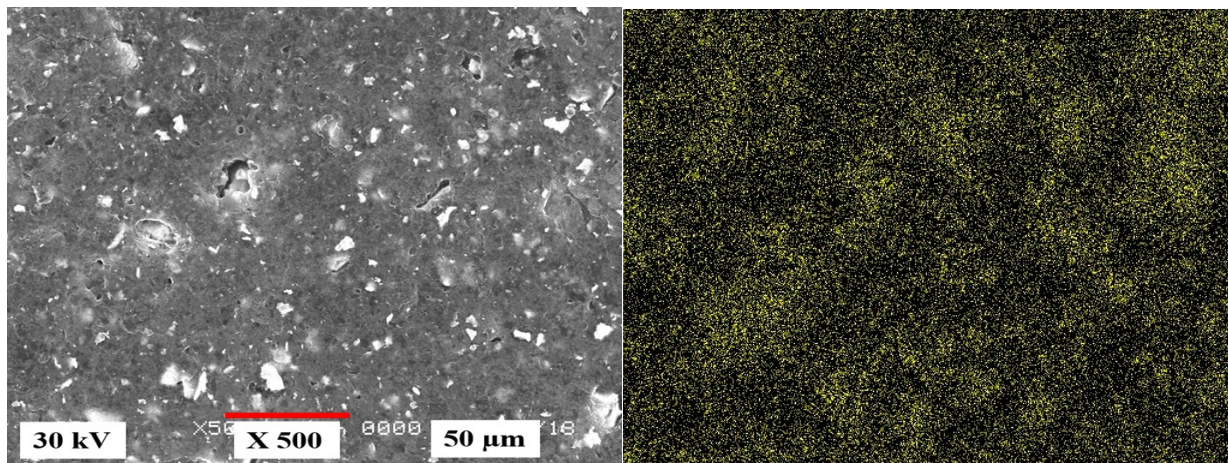
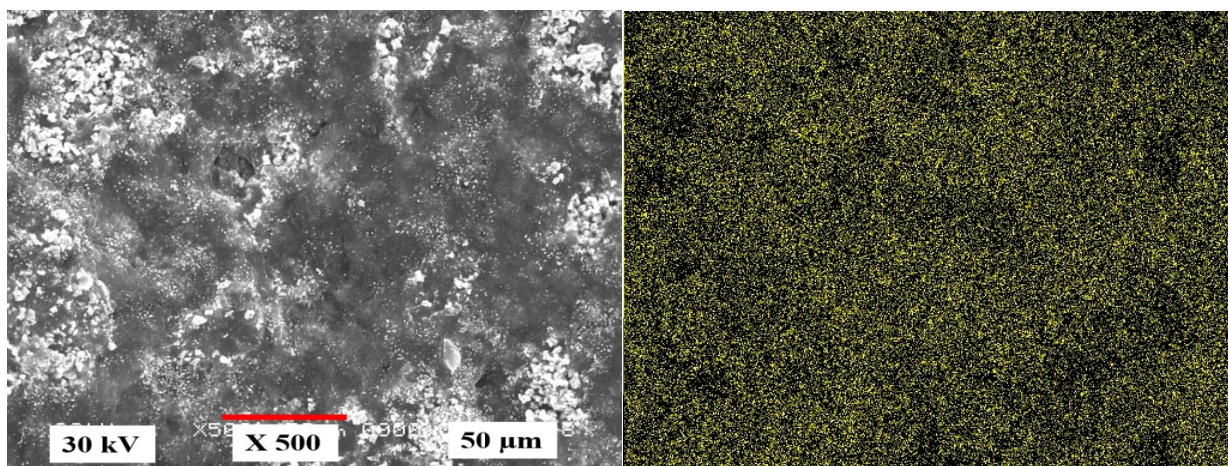


Figure S1 and S2: *Ex situ* XRD patterns of Bi/Sb-LiBH₄-AB composite electrodes at different stages (indicated in fig. 2a and 2b) of the first electrochemical discharge – charge process.

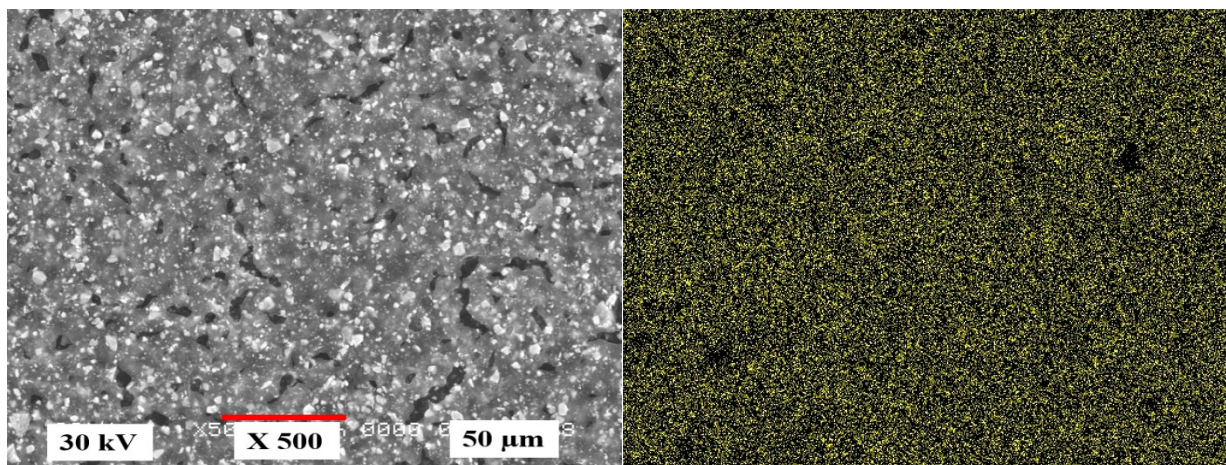


(a)

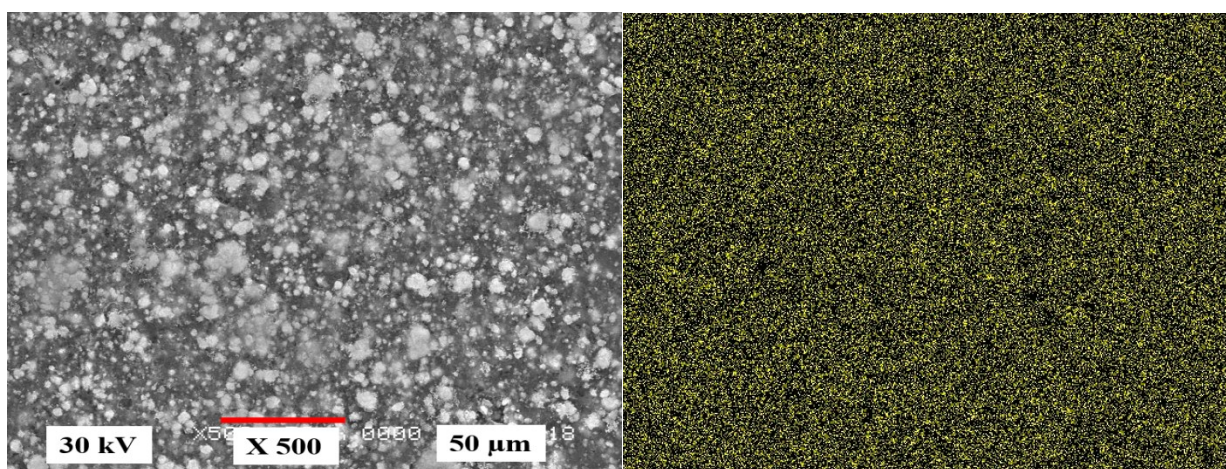


(b)

Figure S₃: SEM images and corresponding elemental (Bi) mapping of Bi-LiBH₄-AB composite electrode (a) before and (b) after cycling.



(a)



(b)

Figure S₄: SEM images and corresponding elemental (Sb) mapping of Sb-LiBH₄-AB composite electrode (a) before and (b) after cycling.