

Carbon-Coated Te-Doped Bi₂Se₃ as a Topological Quantum Anode Material for Sodium-Ion Batteries

Anunad Mishra^{1,*}, Urvesh Vala²

Abstract

Sodium-ion batteries (SIBs) are increasingly investigated as cost-effective alternatives to lithium-ion systems for large-scale energy storage; however, the development of stable and conductive anode materials remains a major challenge. In this work, tellurium-doped bismuth selenide (Te-doped Bi₂Se₃) was synthesized and further modified with Super P conductive carbon to improve its sodium-storage behavior. The phase formation and structural retention of the active material were examined using X-ray diffraction, while elemental mapping and energy-dispersive X-ray spectroscopy verified the incorporation of Te and the presence of carbon in the modified sample. Thermogravimetric analysis showed that the material remained thermally stable up to approximately 500°C. Electrochemical testing in sodium half-cells revealed that the uncoated Te-doped Bi₂Se₃ electrode delivered stable capacities of about 150 mAh g⁻¹ at 20 mA g⁻¹ and 110 mAh g⁻¹ at 40 mA g⁻¹. After carbon modification, the corresponding capacities increased to approximately 250 mAh g⁻¹ and 175 mAh g⁻¹, respectively. Cyclic voltammetry further indicated improved redox reversibility and more stable peak currents for the carbon-modified electrode. These results suggest that carbon-coated/composite Te-doped Bi₂Se₃ is a promising anode candidate for SIBs, with carbon modification providing improved conductivity, enhanced reaction reversibility, and better rate performance.

Keywords: Sodium-ion battery, Te-doped Bi₂Se₃, carbon coating, Super P., anode, topological quantum material

INTRODUCTION

The increasing demand for sustainable and affordable energy-storage systems has accelerated the development of battery technologies beyond conventional lithium-ion batteries. Although lithium-ion batteries offer high energy density and long cycle life, concerns related to lithium availability, raw-material cost, and supply-chain limitations have encouraged the exploration of alternative rechargeable battery chemistries. Sodium-ion batteries are particularly attractive because sodium is abundant, low-cost, and chemically similar to lithium, allowing the transfer of several design concepts from lithium-ion systems to sodium-based cells [1-3].

Despite these advantages, SIBs face important materials challenges. The larger ionic radius and higher atomic mass of Na⁺ compared with Li⁺ can lead to slower ion diffusion, larger structural strain, and poor cycling stability in many conventional electrode materials. Therefore, suitable anode materials for SIBs must combine high sodium-storage capacity, good electronic conductivity, structural stability, electrolyte compatibility, and resistance to volume-change-induced degradation [4-5]. Conventional carbonaceous and alloying anodes often suffer from limited capacity, sluggish kinetics, or pronounced mechanical degradation during repeated sodiation and desodiation.

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Layered chalcogenide materials, including bismuth selenide (Bi₂Se₃), are interesting candidates for sodium-ion storage because of their layered crystal structure, relatively high density, and favorable electronic properties.[6] Bi₂Se₃ is also widely recognized as a topological quantum material, and its robust electronic structure can support efficient charge transport. Doping provides an additional route for tuning the lattice and electronic structure. In particular, Te incorporation into Bi₂Se₃ can modify the electronic environment, potentially enhance charge-transfer behavior, and improve structural stability during repeated cycling [7-8].

However, Te-doped Bi₂Se₃ alone may still experience irreversible reactions and unstable capacity during electrochemical cycling, partly due to interfacial side reactions and the formation of irreversible sodium-containing compounds such as Na₂Se or Na₂Te during the initial cycles. Carbon modification is a practical strategy to address these limitations. Conductive carbon can improve electronic pathways, promote better electrode integrity, and buffer local strain during Na⁺ insertion/extraction [9]. In this study, 10 wt% Te-doped Bi₂Se₃ was synthesized and modified with Super P carbon. The structural, compositional, thermal, and electrochemical properties of uncoated and carbon-modified electrodes were compared to evaluate the role of carbon coating/composite formation in improving sodium-storage behavior [10].

EXPERIMENTAL SECTION

Synthesis of Te-Doped Bi₂Se₃

Te-doped Bi₂Se₃ was prepared using a modified Bridgman-type route. High-purity Bi, Se, and Te precursors were weighed according to the target composition of Bi₂Se_{3-x}Te_x with 10 wt% Te doping. The powders were mixed and ground thoroughly to obtain a homogeneous precursor mixture and then pressed into pellets under an argon-filled glovebox atmosphere to minimize oxidation and contamination. The pellets were sealed in a quartz ampoule, evacuated to approximately 10⁻⁵ Pa, and subjected to a controlled heat treatment. The ampoule was heated to 850°C for 12 h, cooled to 620°C at 2°C h⁻¹, further cooled to 550°C at 5°C h⁻¹, held at 550°C for 72 h, and finally cooled to room temperature at 20°C h⁻¹.

Carbon Modification Using Super P

For carbon modification, the synthesized Te-doped Bi₂Se₃ powder was dispersed and stirred at 750 rpm for 2 h. Separately, Super P conductive carbon black was dispersed in a deionized water/ethanol solvent mixture and stirred at 750 rpm for 2 h to improve dispersion and reduce carbon agglomeration. The two suspensions were then combined and treated by mechanical stirring together with probe-assisted ultrasonication for an additional 2 h. The resulting mixture was transferred to a Teflon-lined stainless-steel autoclave and hydrothermally treated at 160°C for 12 h. After natural cooling, the product was washed and dried to obtain carbon-modified Te-doped Bi₂Se₃.

Electrode Preparation and Cell Assembly

Working electrodes were prepared by mixing active material, conductive carbon, and polyvinylidene fluoride (PVDF) binder in an 8:1:1 mass ratio. N-methyl-2-pyrrolidone (NMP) was used as the solvent to form a uniform slurry. The slurry was cast onto a metallic current collector and dried at 40°C overnight, followed by vacuum drying at 40°C for 48 h. Circular electrodes of approximately 13 mm diameter were punched from the dried sheet. Sodium half-cells were assembled in CR-type coin cells inside an argon-filled glovebox using sodium metal as the counter/reference electrode, a separator soaked with electrolyte, and the prepared Te-doped Bi₂Se₃-based electrode as the working electrode. The same fabrication route was used for both uncoated and carbon-modified electrodes as given in Figure 1.

Characterization and Electrochemical Measurements

The crystalline phase was examined by X-ray diffraction (XRD), and the elemental distribution was analyzed using scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy

(SEM–EDS). Thermal stability was evaluated by thermogravimetric analysis (TGA). Cyclic voltammetry (CV) was conducted at a scan rate of 0.1 mV s^{-1} within the tested voltage range. Galvanostatic charge–discharge measurements were performed at different current densities, including 10, 20, 40, and 100 mA g^{-1} , to evaluate rate capability, specific capacity, cycling stability, and Coulombic efficiency.

RESULTS AND DISCUSSION

Structural and Compositional Analysis

Figure 2 compares the XRD patterns of uncoated and carbon-modified Te-doped Bi_2Se_3 . The uncoated sample shows characteristic diffraction peaks corresponding to rhombohedral Bi_2Se_3 , consistent with the JCPDS reference pattern 00-033-0214. Dominant reflections indexed to the (00 3n) family, along with a minor (015) peak, indicate the formation of the layered Bi_2Se_3 -based structure. After carbon modification, the main Bi_2Se_3 reflections are retained, suggesting that the carbon-treatment process does not destroy the host crystal structure. The slight changes in relative intensity and minor deflections may be attributed to the presence of carbon and interfacial interaction between Super P and the Te-doped Bi_2Se_3 particles. EDS elemental mapping confirms the distribution of Bi, Se, and Te in the synthesized material, supporting the successful incorporation of Te into the Bi_2Se_3 -based structure. For the carbon-modified sample, EDS spectra show the presence of carbon in addition to Bi, Se, and Te, verifying the formation of a carbon-containing composite/coated electrode material. This carbon phase is expected to provide improved electrical connectivity between active particles and reduce charge-transfer limitations during sodium-ion storage as shown in Figure 3.



Figure 1. Glove box setup for coin cell preparation.

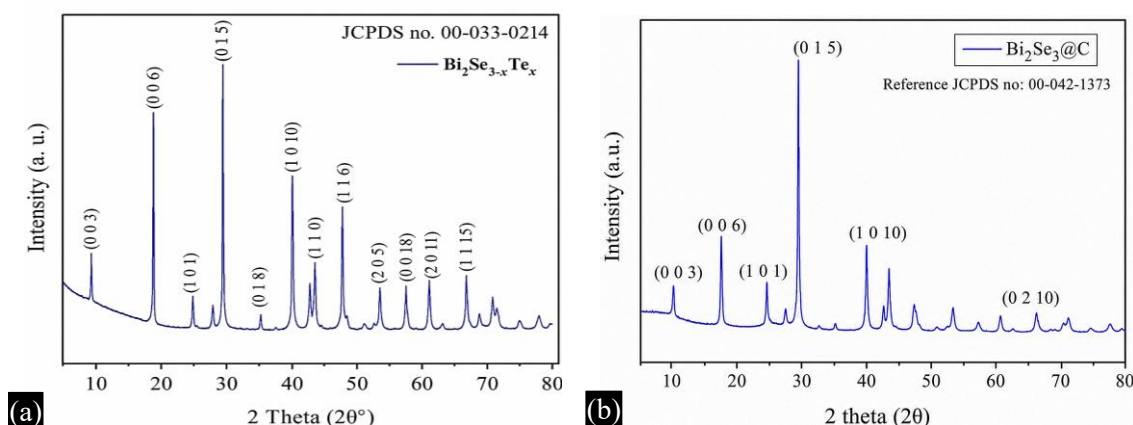
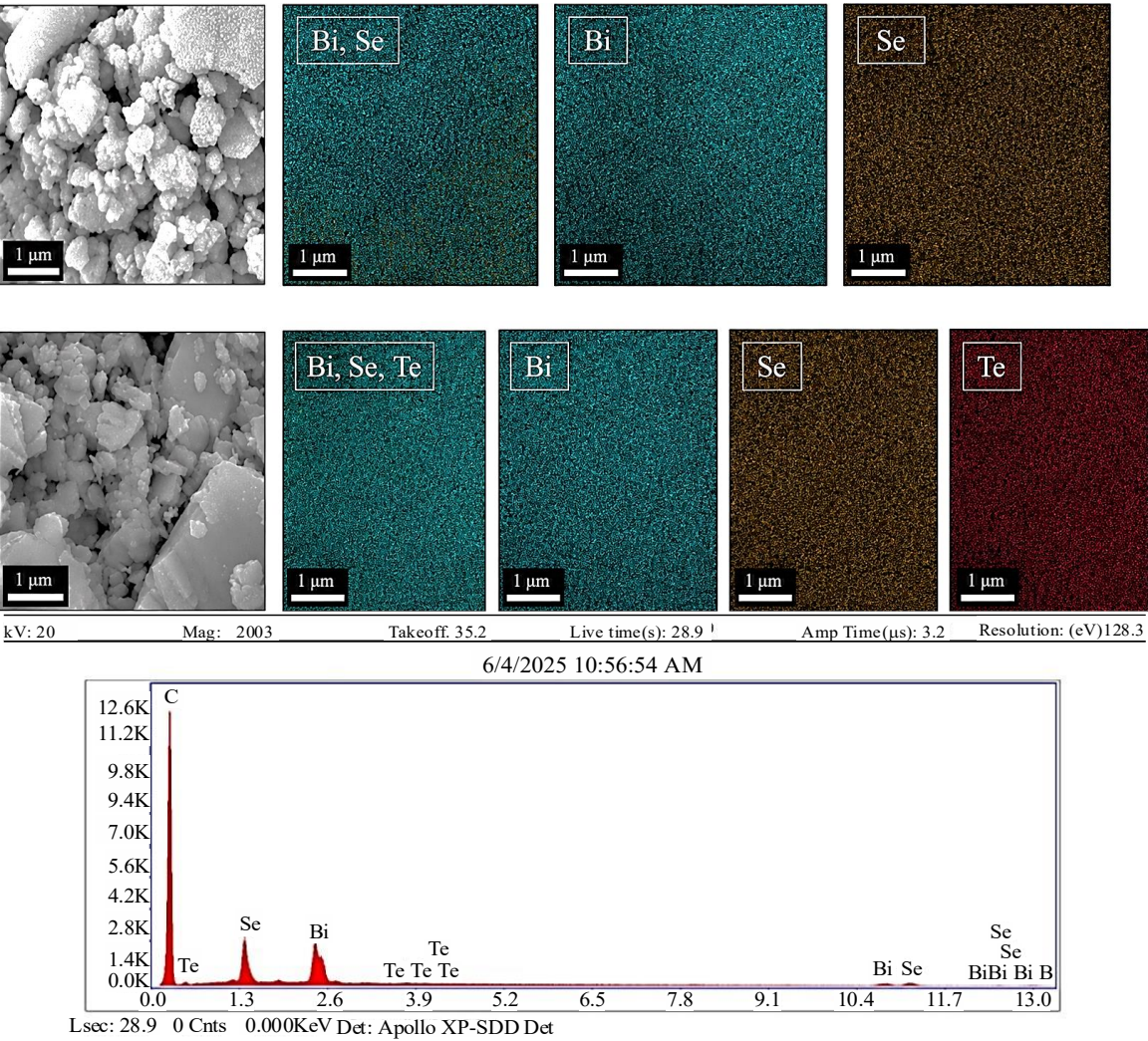


Figure 2. (a, b) XRD patterns of uncoated Te-doped Bi₂Se₃ and carbon-modified Te-doped Bi₂Se₃



eZAF Smart quant results									
Element	Weight %	Atomic %	Net intensity	Error %	K-ratio	Z	R	A	F
Carbon (C K)	85.3	98.2	3002.3	5.8	0.4898	1.0485	0.9619	0.5474	1.0000
Bismuth (Bi M)	7.0	0.5	549.3	6.6	0.0594	0.5922	1.4429	1.3629	1.0527
Tellurium (Te L)	0.1	0.0	5.5	58.6	0.0008	0.6322	1.2585	1.1213	1.0078
Selenium (Se K)	7.5	1.3	66.3						

Figure 3. EDS mapping and spectra confirming Te incorporation and carbon presence after Super P modification.

Thermal Stability

The TGA profile of Te-doped Bi₂Se₃ indicates that the synthesized material remains thermally stable up to approximately 500°C. Above this temperature, measurable weight loss is observed, which can be associated with decomposition, oxidation, or bond-breaking processes at elevated temperature. The stability up to 500°C is favorable for electrode-processing and battery-operation considerations, as it suggests that the active material can withstand thermal exposure far above typical room-temperature electrochemical testing conditions in Figure 4.

Cyclic Voltammetry

Cyclic voltammetry was used to investigate the redox behavior of the Te-doped Bi_2Se_3 electrodes during sodium insertion and extraction. The uncoated Te-doped Bi_2Se_3 electrode shows cathodic and anodic features associated with sodiation and desodiation reactions. During the early cycles, the peak shape and intensity vary, indicating activation of the electrode and the occurrence of irreversible reactions. The CV curves become more stable after approximately the fourth cycle, suggesting partial stabilization of the electrode/electrolyte interface. The asymmetry between cathodic and anodic features in the uncoated electrode indicates incomplete reversibility, which may be related to irreversible formation of sodium selenide/telluride species and interfacial side reactions.

In contrast, the carbon-modified Te-doped Bi_2Se_3 electrode exhibits more symmetric redox peaks, higher peak currents, and improved overlap of successive cycles. These features indicate enhanced electrochemical reversibility and faster charge-transfer kinetics. The conductive Super P network likely improves electron transport and helps maintain electrical contact between active particles during repeated sodiation/desodiation. Therefore, carbon modification plays a direct role in stabilizing the electrode response and reducing polarization during cycling in Figure 5 and Figure 6.

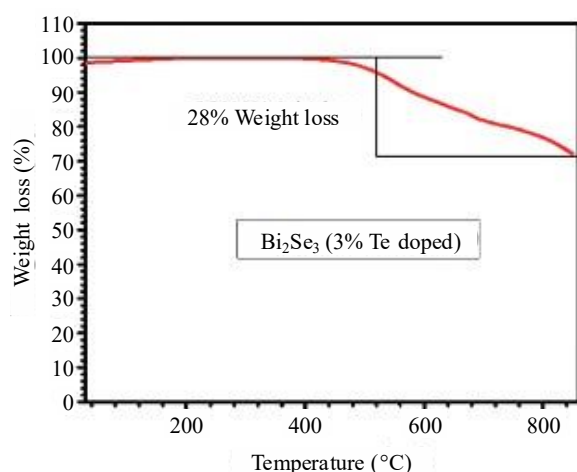


Figure 4. TGA curve showing thermal stability of Te-doped Bi_2Se_3 up to approximately 500°C.

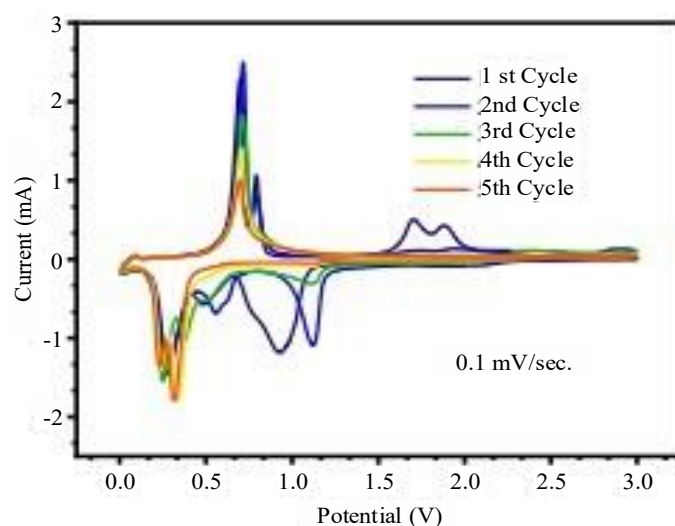


Figure 5. CV curves of uncoated Te-doped Bi_2Se_3 electrodes at 0.1 mV s⁻¹.

Charge–Discharge Performance

Galvanostatic charge–discharge testing further demonstrates the beneficial effect of carbon

modification. For the uncoated Te-doped Bi₂Se₃ electrode, the stable fifth-cycle capacity is approximately 250 mAh g⁻¹ at 10 mA g⁻¹. When the current density increases to 20 mA g⁻¹ and 40 mA g⁻¹, the stable capacities decrease to about 150 mAh g⁻¹ and 110 mAh g⁻¹, respectively. This reduction at higher current densities reflects kinetic limitations, incomplete Na⁺ diffusion, and increased polarization in the uncoated electrode as shown in Figure 7.

The carbon-modified Te-doped Bi₂Se₃ electrode shows significantly improved capacity retention at higher current densities. At 20 mA g⁻¹, the coated/composite electrode delivers a stable capacity of approximately 250 mAh g⁻¹, which is higher than the 150 mAh g⁻¹ obtained for the uncoated sample under the same condition. At 40 mA g⁻¹, the carbon-modified electrode maintains approximately 175 mAh g⁻¹, compared with 110 mAh g⁻¹ for the uncoated electrode. These improvements confirm that carbon modification enhances the rate capability of Te-doped Bi₂Se₃ by improving electronic conductivity and preserving electrode integrity during cycling as given in Figure 8.

Cycling Stability and Coulombic Efficiency

The cycling behavior of the carbon-modified electrode at 100 mA g⁻¹ shows an initial stabilization period, during which Coulombic efficiency remains around 90–95%. This initial inefficiency can be attributed to irreversible reactions, formation of interfacial layers, and electrode activation. After stabilization, the Coulombic efficiency approaches approximately 100%, indicating improved reversibility of sodium insertion/extraction. Although capacity decreases at higher current densities compared with lower-current testing, the stable Coulombic efficiency confirms that the carbon-modified electrode can sustain repeated cycling after activation. Further optimization of coating uniformity, particle size, electrolyte composition, and electrode mass loading may improve the long-term capacity retention.

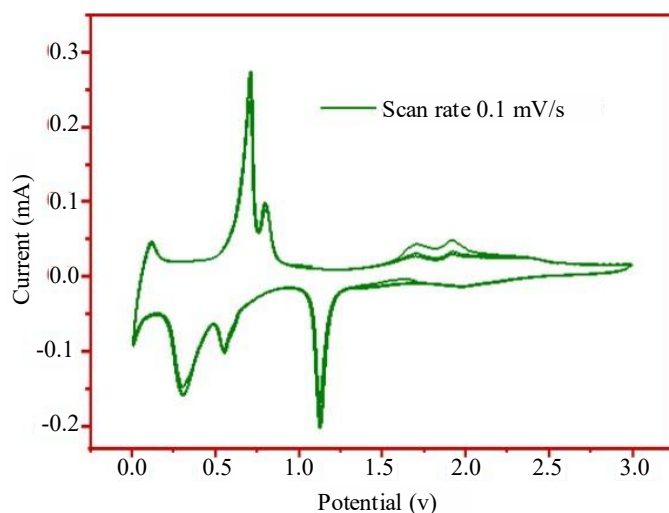


Figure 6. CV curves of carbon-modified Te-doped Bi₂Se₃ electrodes at 0.1 mV s⁻¹.

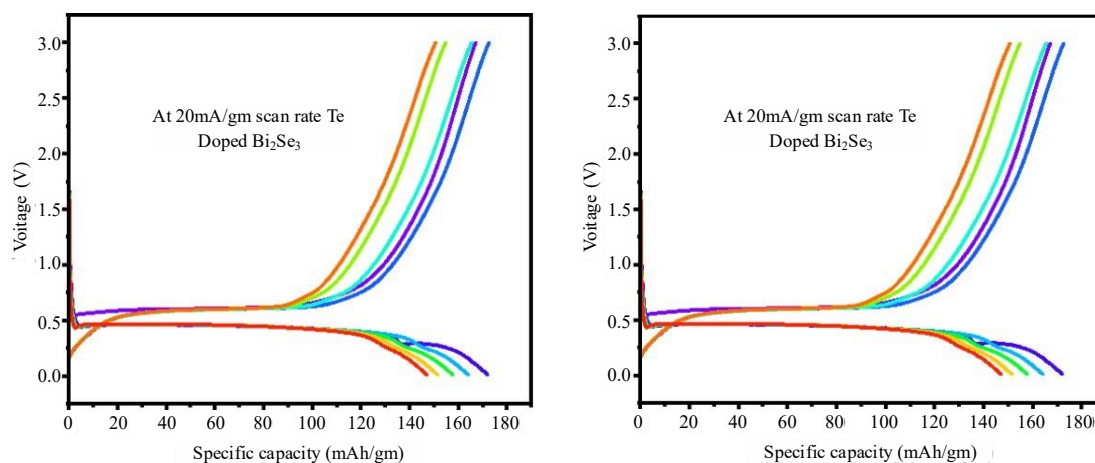


Figure 7. (a, b) Galvanostatic charge–discharge behavior of uncoated Te-doped Bi_2Se_3 electrodes at different current densities.

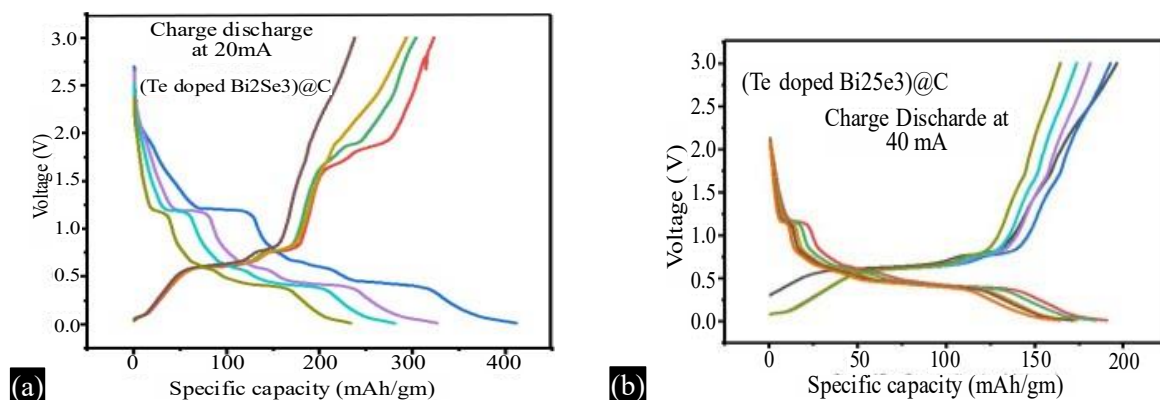


Figure 8. (a, b) Galvanostatic charge–discharge behavior of carbon-modified Te-doped Bi_2Se_3 electrodes at different current densities.

CONCLUSION

Te-doped Bi_2Se_3 and carbon-modified Te-doped Bi_2Se_3 were prepared and evaluated as anode materials for sodium-ion batteries. XRD confirmed the formation and structural retention of the Bi_2Se_3 -based phase, while EDS verified Te incorporation and carbon presence in the modified sample. TGA showed thermal stability up to approximately 500 °C. Electrochemical analysis demonstrated that carbon modification improved redox reversibility and rate performance compared with the uncoated electrode. The uncoated sample delivered stable capacities of approximately 150 mAh g^{-1} at 20 mA g^{-1} and 110 mAh g^{-1} at 40 mA g^{-1} , while the carbon-modified electrode delivered approximately 250 mAh g^{-1} and 175 mAh g^{-1} under the same respective current densities. Coulombic efficiency approached ~100% after initial stabilization, indicating improved reversibility. Overall, carbon-coated/composite Te-doped Bi_2Se_3 is a promising anode material for sodium-ion batteries, and further optimization of the carbon architecture and electrode/electrolyte interface may lead to improved long-term cycling stability.

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