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Supplementary Information:

Layered Sb_2Te_3 and its nanocomposite: A new and outstanding electrode material for superior rechargeable Li-ion batteries

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Experimental

Materials Synthesis: Sb_2Te_3 was synthesized by the following solid-state synthetic processes. Stoichiometric amounts of Sb (Sigma-Aldrich, average size: ca. 50 μm, 99.98%) and Te (Sigma-Aldrich, average size: ca. 100 μm, 99.5%) powders, and stainless steel balls (diameter: 3/8 in. and 3/16 in.) were placed in a hardened steel vial (80 cm^3) with a ball-to-powder ratio of 20:1. The high-energy ball milling (HEBM, Spex-8000) process was conducted under an Ar atmosphere for 6 h. To obtain the Sb_2Te_3/C nanocomposite, an additional HEBM process was applied to the mixture of Sb_2Te_3 and carbon black (Super P) powders. Preliminary electrochemical tests were selected on the basis of the electrochemical performances, such as initial capacity, initial coulombic efficiency, and cycling performance. The optimum amounts of Sb_2Te_3 and C were 60 and 40 wt%, respectively.

Materials Characterization: The structure of the active material powders was characterized by X-ray diffraction (XRD, DMAX2500-PC, Rigaku), high-resolution transmission electron microscopy (HRTEM, FEI F20, operating at 200 kV), and energy-dispersive spectroscopy (EDS, attached to the HRTEM). *Ex situ* XRD and TEM analyses were used to observe the structural changes occurring in the active material of Sb_2Te_3 and the Sb_2Te_3/C composite electrodes during cycling.

Electrochemical Measurements: The Sb_2Te_3 and Sb_2Te_3/C powders were mixed with carbon black (Denka) and polyvinylidene fluoride (PVDF) dissolved in N-methyl-2-pyrrolidone (NMP) to form a slurry at a ratio of 80:10:10. Coin-type electrochemical cells were assembled in an argon-filled glove box using a separator (Celgard 2400), Li foil as the counter and reference electrodes, and 1 M $LiPF_6$ in ethylene carbonate/diethyl carbonate (EC/DEC, 1:1 by volume, Pannax STARLYTE) as the electrolyte. With the exception of the rate-capability tests, all cells were galvanostatically tested between 0.0 and 3.0 V (vs. Li^+/Li) at a current density of 100 mA g^{-1} using a Maccor automated tester. Cyclic voltammograms (CVs) were recorded using a ZIVE MP2A with voltages ranging from 0 to 3 V under a scan rate of 0.15 mV s^{-1}. Li was inserted into the electrode during discharging and was extracted from the working electrode during charging. The gravimetric capacity was calculated on the basis of the weight of the active materials, and the volumetric capacity was calculated by multiplying the gravimetric capacity by the tap density (Sb_2Te_3: 3.68 g cm^{-3}, Sb_2Te_3/C composite: 2.05 g cm^{-3}, and MCMB graphite: 1.27 g cm^{-3}), which was measured using a powder tap density tester (BT-301, Bettersize).

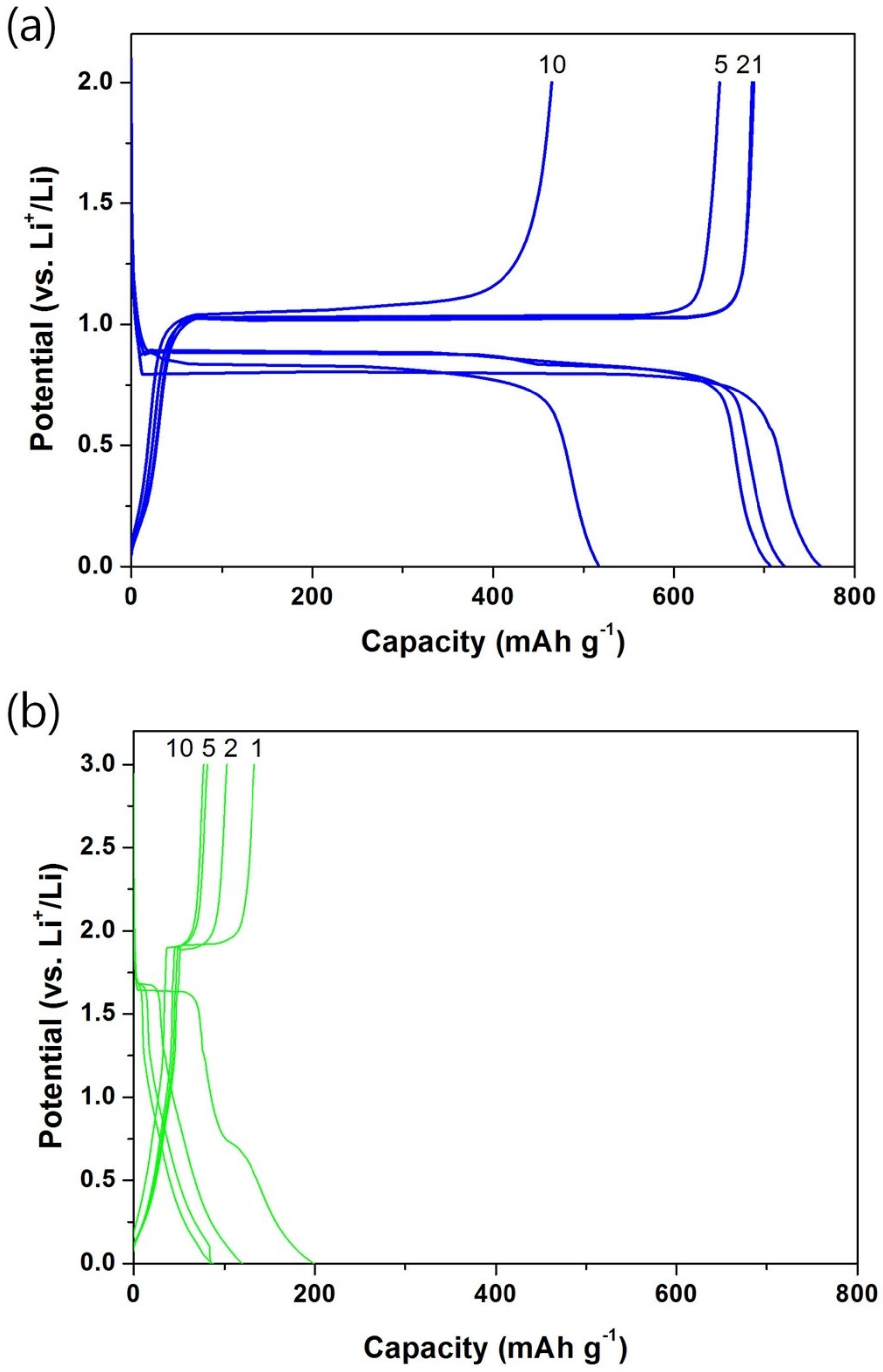

Figure S1. Electrochemical performances of the Sb and Te electrodes: (a) Voltage profile of the Sb electrode and (b) voltage profile of the Te electrode.

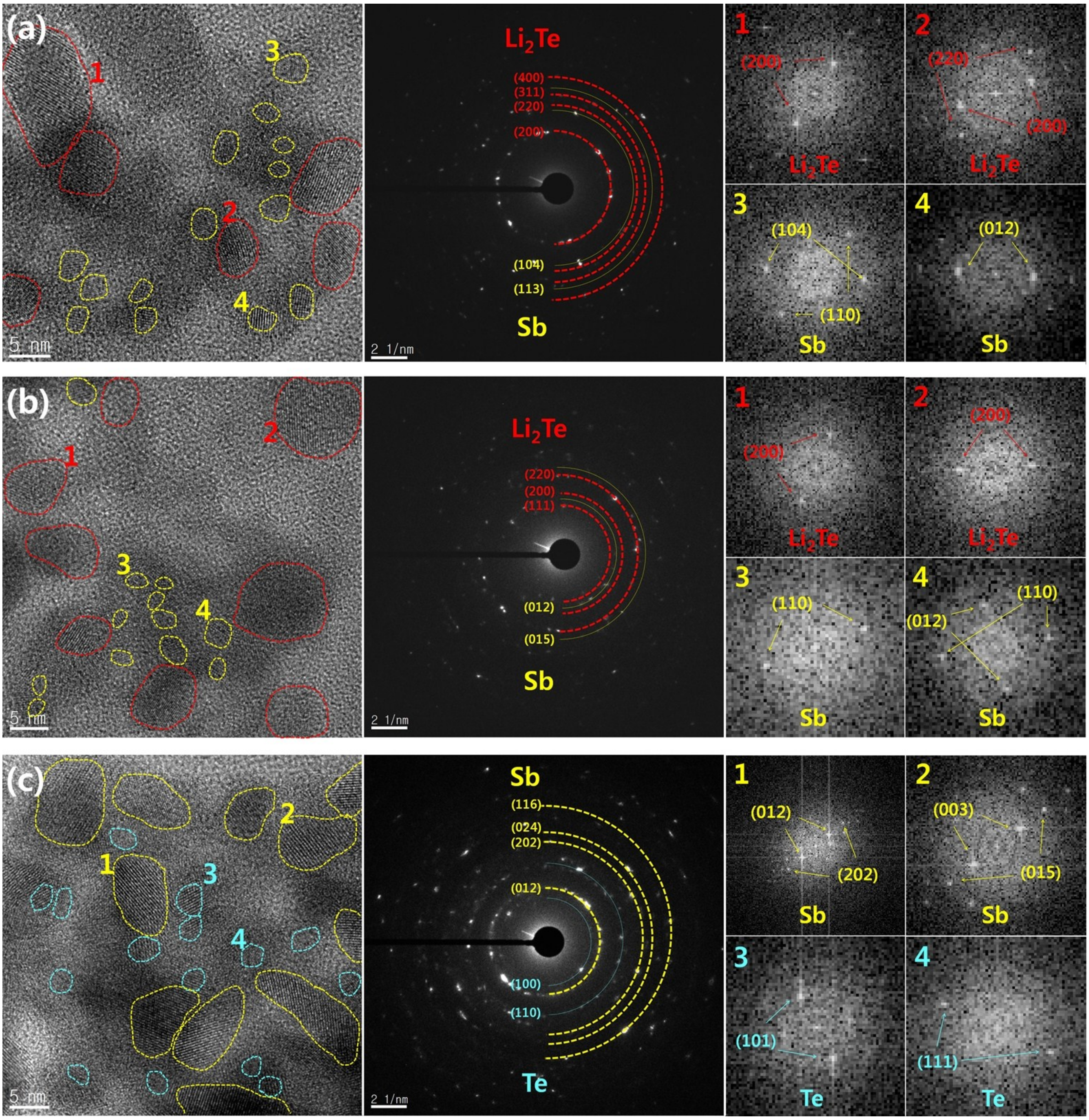

Figure S2. *Ex situ* HRTEM results of the Sb_2Te_3 electrode. (a) *Ex situ* HRTEM result of discharged state at 1.0 V (t_1 in Fig. 1c) with corresponding FT patterns, (b) *Ex situ* HRTEM result of charged state at 1.5 V with (t_3 in Fig. 1c) corresponding FT patterns, and (c) *Ex situ* HRTEM result of fully discharged state at 3.0 V (t_4 in Fig. 1c) with corresponding FT patterns.

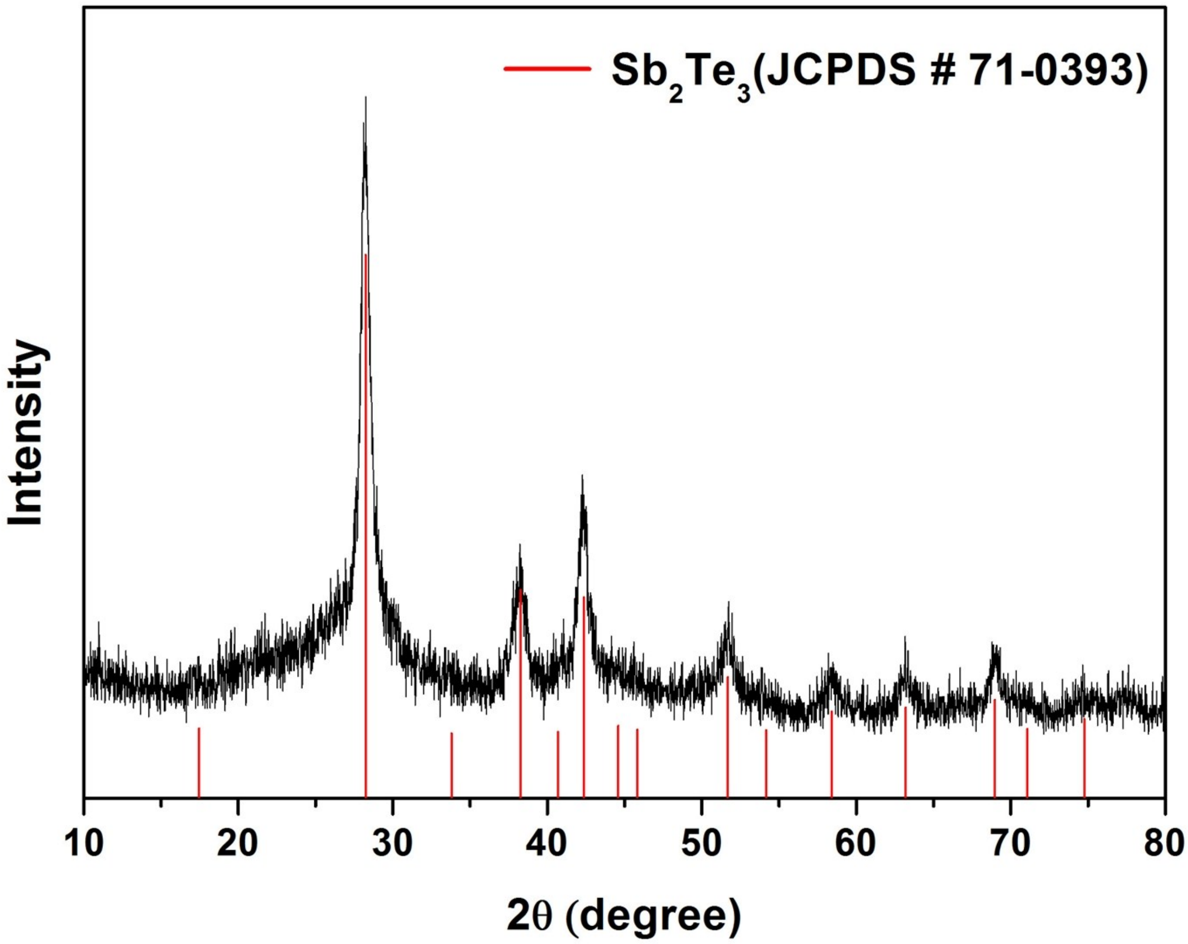

Figure S3. XRD pattern of the Sb_2Te_3/C composite prepared by an additional HEBM process.

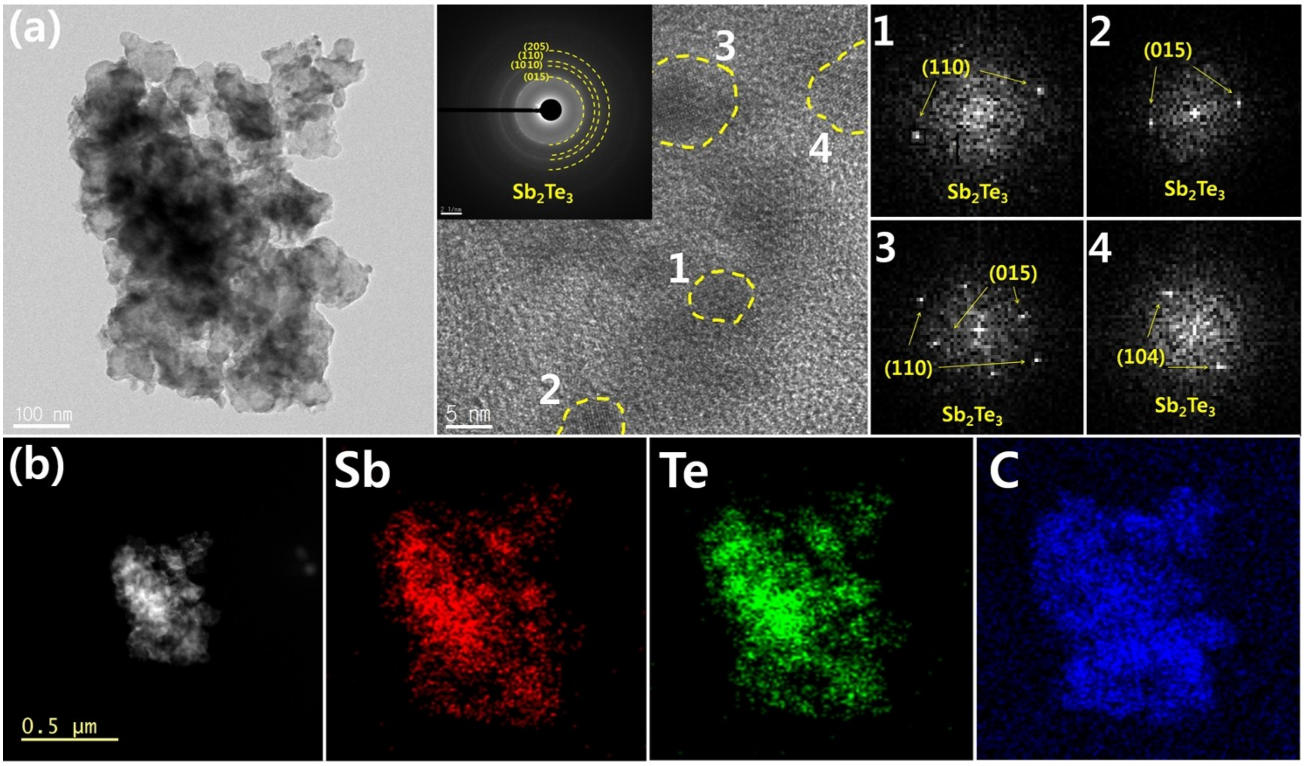

Figure S4. HRTEM results for the Sb_2Te_3/C composite: (a) Bright-field TEM and HRTEM images combined with corresponding FT patterns and (b) STEM image and its corresponding EDS mapping images.

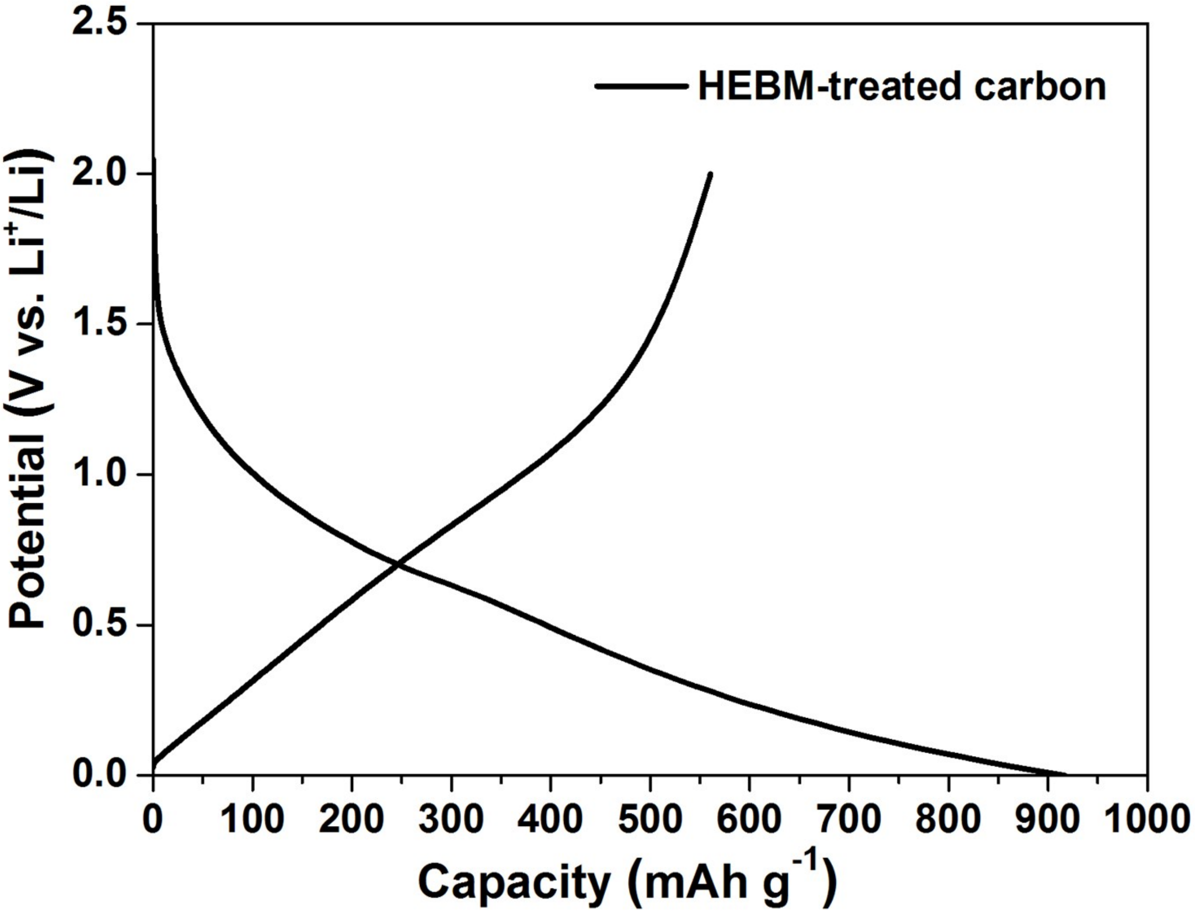

Figure S5. Voltage profile of the HEBM-treated carbon (Super P). electrode (voltage range from 0 to 2.0 V under a current rate of 100 mA g^{-1}).

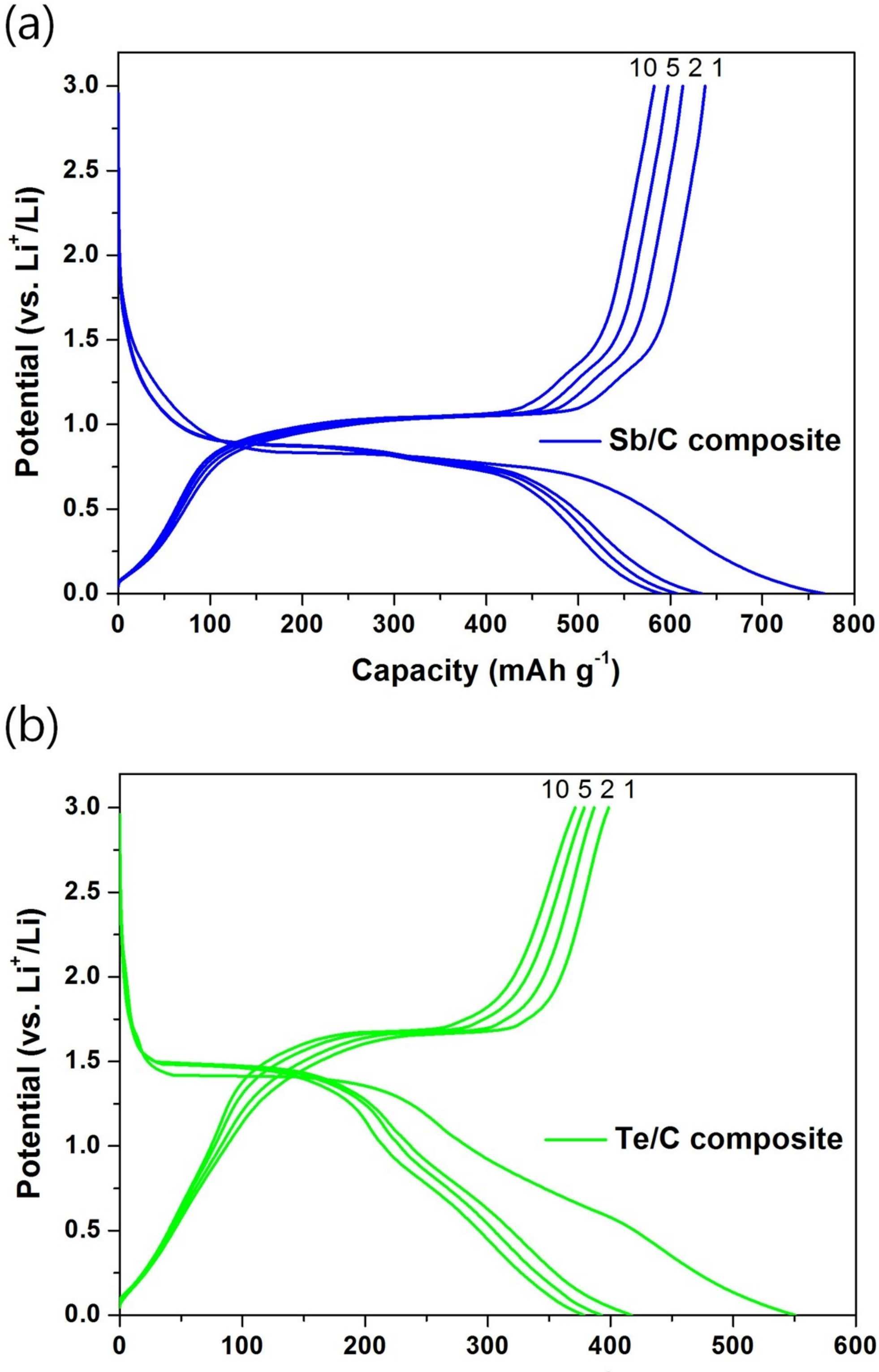

Figure S6. Electrochemical performances of the Sb/C and Te/C composite electrodes: (a) Voltage profile of the Sb/C composite electrode and (b) voltage profile of the Te/C composite electrode (voltage range from 0 to 3 V under a current rate of 100 mA g^{-1}).

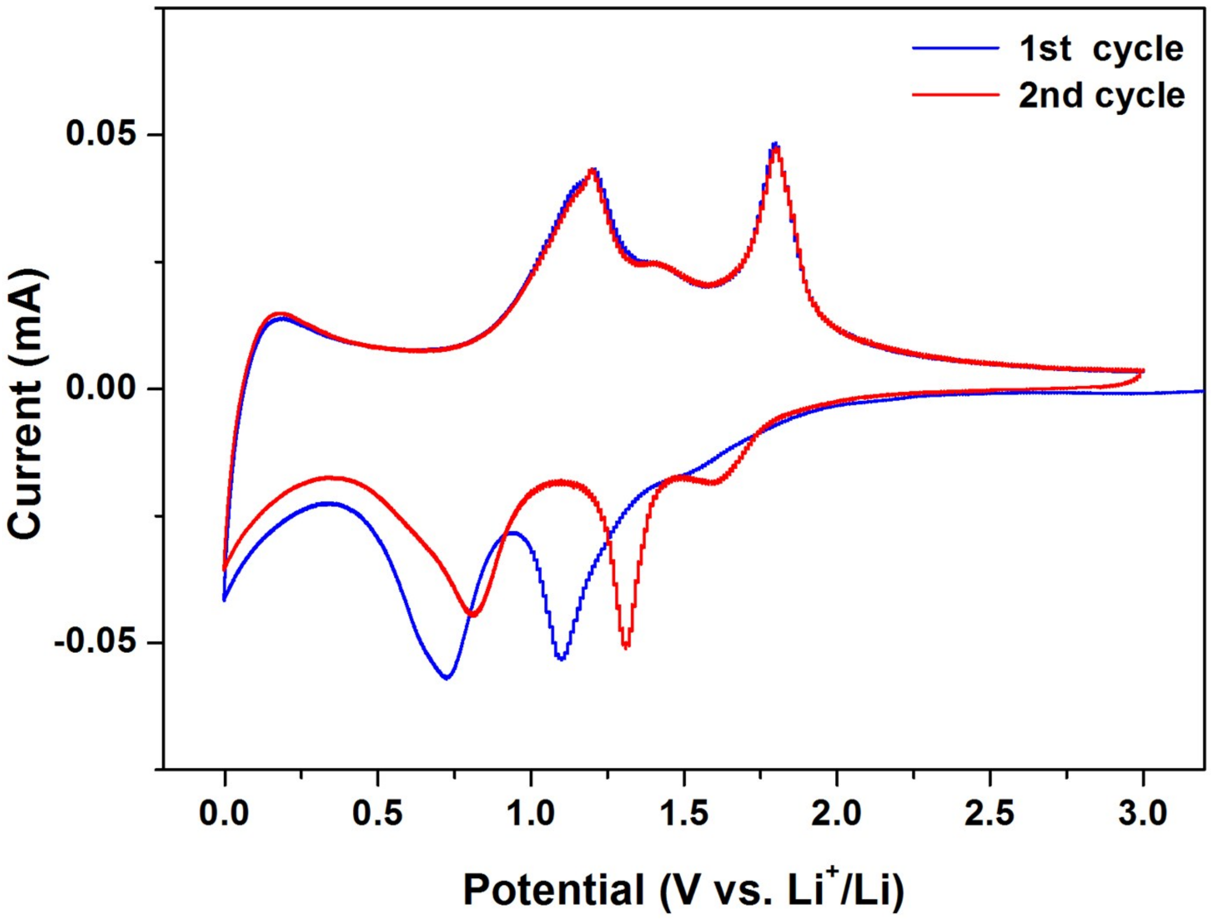

Figure S7. CV results of the first and second cycles for the Sb_2Te_3/C nanocomposite electrode (voltage range from 0 to 3 V under a scan rate of 0.15 mV s^{-1}).

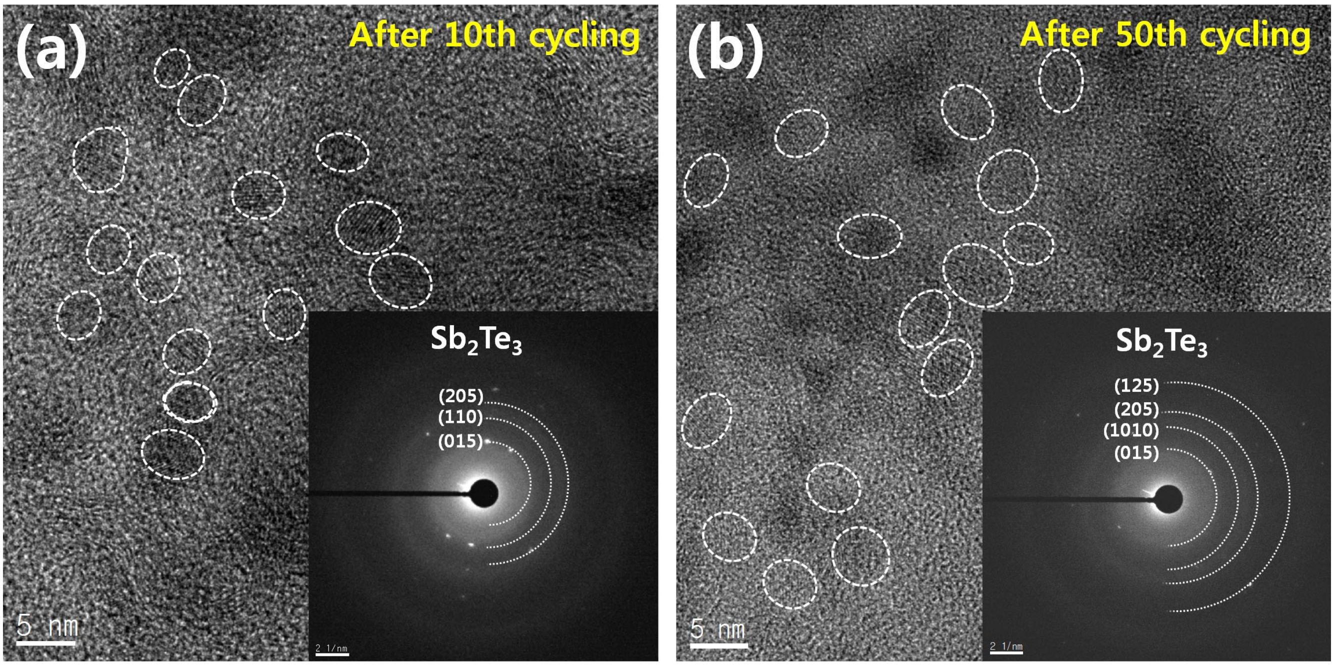

Figure S8. Characterization of Sb_2Te_3 nanocrystallites in Sb_2Te_3/C nanocomposite electrodes. (a) HRTEM image with corresponding diffraction patterns of the Sb_2Te_3/C nanocomposite electrode after the 10th cycling and (b) HRTEM image with corresponding diffraction patterns of the Sb_2Te_3/C nanocomposite electrode after the 50th cycling.

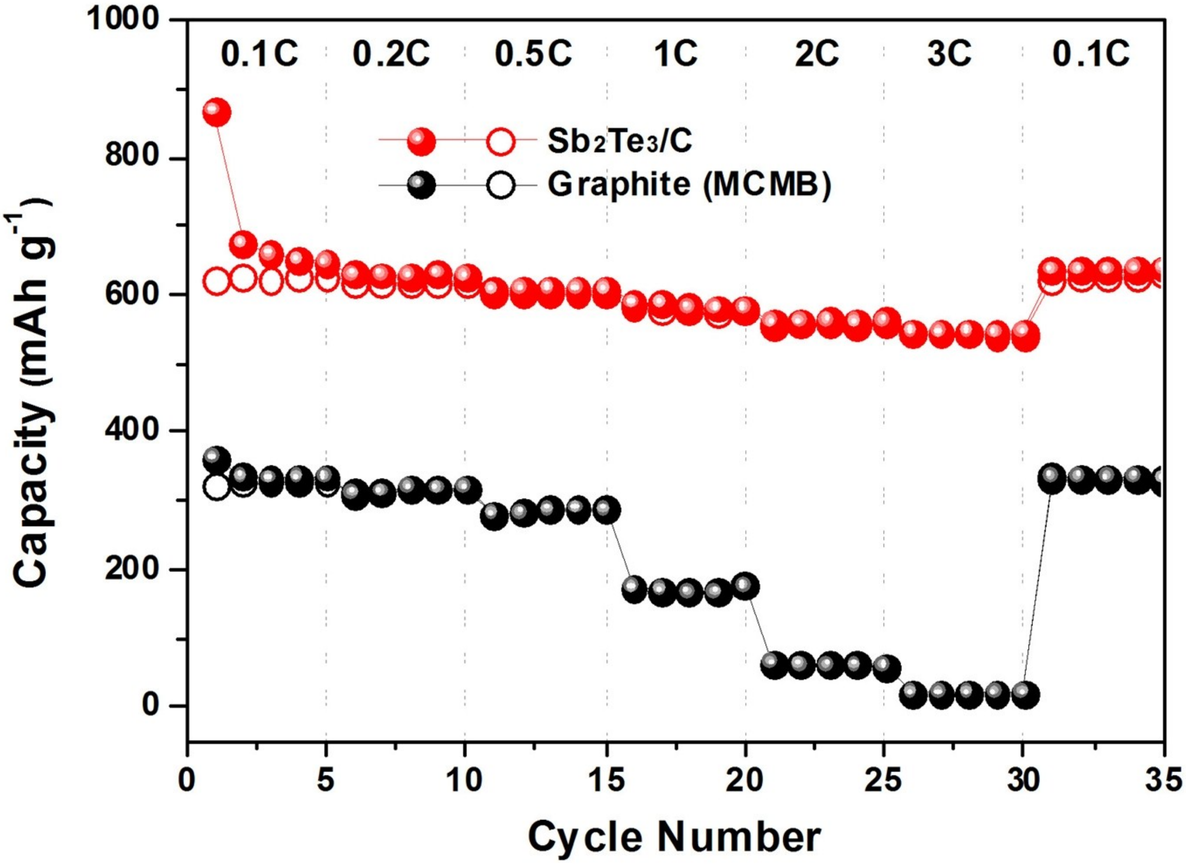

Figure S9. Comparison of the gravimetric capacities at various C-rates for the Sb_2Te_3/C and MCMB electrodes.