

# Correction to Improved Electrochemical Capacity of Precursor-Derived Si(B)CN-Carbon Nanotube Composite as Li-Ion Battery Anode

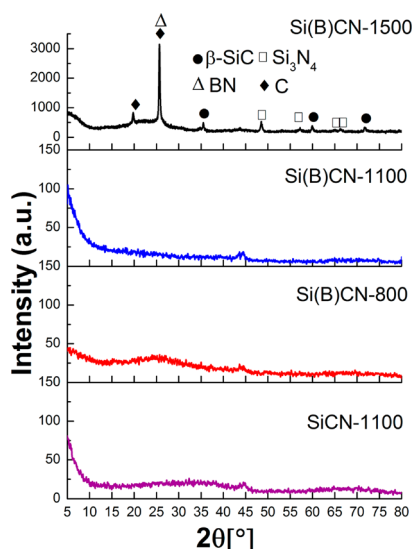
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**P** 5095. The correct values of  $D_{Li}$  for Si(B)CN-CNT are in the range of approximately  $1 \times 10^{-13}$  and  $1 \times 10^{-16}$  m<sup>2</sup>/s during intercalation and extraction. These values are in the same range as polymer-derived SiOC anodes. In addition and related to this, Figure S4b in the Supporting Information was incorrect. The revised Supporting Information is present below in its entirety.

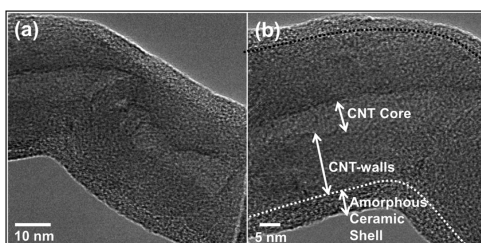
## I. X-RAY DIFFRACTION DATA (XRD)

To characterize the crystalline nature of the specimens processed at higher temperature Bruker powder X-ray diffractometer (Madison, WI) using Cu-K $\alpha$  radiation and nickel filter was employed.



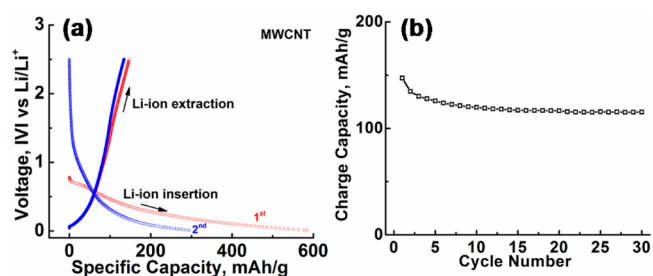
**Figure S1.** X-ray diffraction data for various Si(B)CN and SiCN pellet specimen, confirming the amorphous nature of the precursor-derived Si(B)CN ceramic for temperatures below 1500 °C.

## II. TRANSMISSION ELECTRON MICROSCOPY (TEM)



**Figure S2.** High-resolution TEM images of the Si(B)CN-CNT-1100 composite showing the shell/core morphology.

## III. ELECTROCHEMICAL CYCLING



**Figure S3.** (a) First and second charge/discharge cycles for the MWCNT anode, cycled at 100 mA/g, and (b) Charge capacity for the first 30 cycles for MWCNT anode.

## IV. GALVANOSTATIC INTERMITTENT TITRATION TECHNIQUE (GITT) EXPERIMENT

The solid-state lithium ion diffusion coefficients were determined using

$$D_{\text{GITT}} \approx \frac{4}{\pi\tau} \left( \frac{m_B V_M}{M_B S} \right)^2 \left( \frac{\Delta E_s}{\Delta E_t} \right)^2 \quad (1)$$

Where  $m_B$ ,  $V_M$ ,  $M_B$ , and  $S$  are electrode mass, molar volume, molecular weight and surface area, respectively.  $\tau$  is the time over which the constant current pulse is applied and  $\Delta E_s$  and  $\Delta E_t$  are voltage steps as shown in Figure S4.<sup>1,2</sup>

GITT experiment was carried out on the best performing anode, i.e., Si(B)CN-CNT-1100. A current pulse of 100 mA g<sup>-1</sup> was applied for 15 min followed by a 4 h of relaxation between pulses (until equilibrium is realized) was applied to the electrode for during both lithiation and delithiation. The diffusion coefficient ( $D_{Li}$ ) was thus calculated by taking the weight of active material on anode (2.5 mg), molecular weight (based on XPS elemental composition, 147.8 g/mol), molecular volume (64.2 cm<sup>3</sup>/mol), and surface area (1.6 cm<sup>2</sup>).

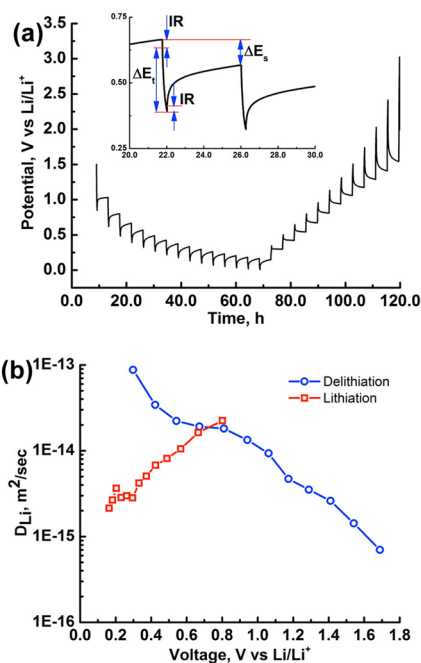
## V. PROCEDURE FOR MEASURING ELECTRICAL RESISTIVITY OF THE PELLETS

Van der Pauw's Four Point Resistivity Measurement Method<sup>3</sup>

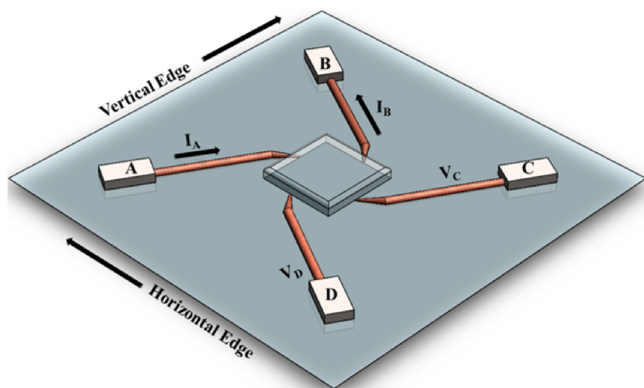
The specimen pellets used for these measurements were formed by cold pressing (4 kpsi) the specimen powder for 30 s without the binder, conducting agent or other additives. The measurements were recorded in the ohmic region.

Step 1: Primary measurement

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**Figure S4.** GITT Data: (a) Charge and discharge cycles with 15 min of current pulse at 100 mA/g followed by 4 h of relaxation for Si(B)CN-CNT-1100 specimen and (b) calculated diffusion coefficient based on the relaxation steps at the corresponding voltages.



**Figure S5.** Experimental setup for measuring the 4-point resistivity measurements.

$R_{AB,CD}$  was defined as the resistance measured with current supplied between points A and B and consequently measuring the potential across points C and D. According to the Ohm's law  $R_{AB,CD}$  was found to be

$$R_{AB,CD} = V_D - V_C / i_{AB} \quad (2)$$

Similarly

$$R_{BC,DA} = V_A - V_D / i_{BC} \quad (3)$$

Step 2: Reciprocal measurements

Ideally as  $R_{AB,CD} = R_{CD,AB}$ , the resistances measured along the edges of the samples were averaged for higher accuracy. Hence

$$R_{edge1} = (R_{AB,CD} + R_{CD,AB}) / 2 \quad (3a)$$

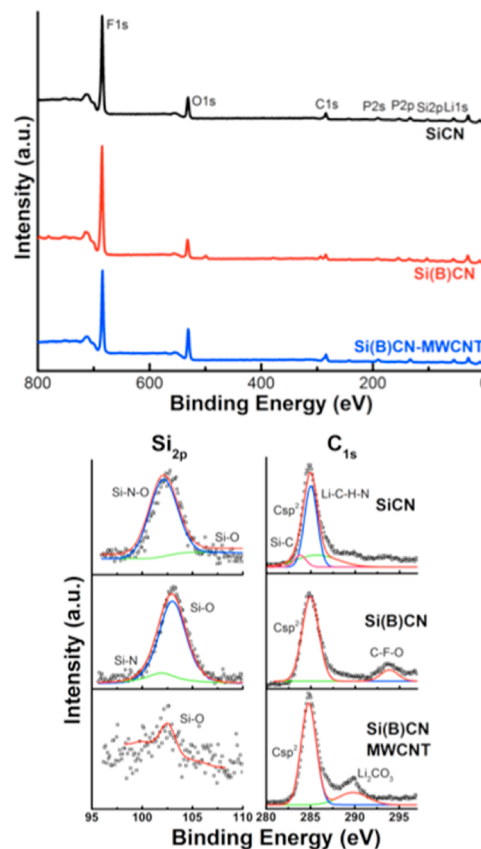
and

$$R_{edge2} = (R_{BC,DA} + R_{DA,BC}) / 2 \quad (4)$$

Step 3: Reverse polarity measurements

**Table S1.** Summary of Surface Elemental Composition of Various Specimen (atomic percent) Used in This Study. All Atomic Percentage Measurements Are Accurate up to Approximately 15%

specimen	Si	B	C	N	O
Si(B)CN-800	24.9	4.6	32.4	19.8	18.4
Si(B)CN-1100	24.4	6.1	24.6	19.5	25.4
Si(B)CN-1500	23.2	5.5	19.7	14.3	37.4
Si(B)CN-CNT-800	13.8	18.2	37.1	17.8	13
Si(B)CN-CNT-1100	9.9	6.5	52.9	2.9	27.7
Si(B)CN-CNT-1500	7.9	17.7	39.9	27	7.5



**Figure S6.** (a) Elemental survey (top) and (b) high-resolution scan (bottom) for SiCN-1100, Si(B)CN-1100, and Si(B)CN-CNT cycled anode specimens.

For attaining higher precise measurements, the polarity at each points were reversed both at the current source and voltage measurement terminals. Hence

$$R_{edge1} = (R_{AB,CD} + R_{BA,DC} + R_{CD,AB} + R_{DC,BA}) / 4 \quad (5)$$

and

$$R_{edge2} = (R_{BC,DA} + R_{CB,AD} + R_{DA,BC} + R_{AD,CB}) / 4 \quad (6)$$

Finally, for the known thickness of the sample  $d$ , the resistivity is defined as

$$\rho = \left( \frac{\pi}{\ln} \right) \left( \frac{d}{2} \right) \frac{R_{edge1} + R_{edge2}}{2} f \quad (7)$$

Where  $f$  is defined as the function of the measured resistances.

## VI. X-RAY PHOTOELECTRON SPECTROSCOPY

Chemical composition on the surface of the specimens was analyzed by X-ray photoelectron spectroscopy using PHI Quantera SXM (Physical Electronics Inc. Chanhassen, MN) with monochromatic Al K $\alpha$  X-radiation (beam size <9  $\mu\text{m}$ ).

### ■ REFERENCES

- (1) Van der Pauw, L. J. *Philips Res. Repts.* **1958**, *13* (1), 1–9.
- (2) Weppner, W.; Huggins, R. J. *Electrochem. Soc.* **1977**, *124* (10), 1569–1578.
- (3) Wen, C.; Boukamp, B.; Huggins, R.; Weppner, W. J. *Electrochem. Soc.* **1979**, *126* (12), 2258–2266.