**Supporting Information**

# Electrochemical performance and stress distribution of $Sb/Sb_2O_3$ nanoparticles as anode materials for sodium-ion batteries

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**Material synthesis and characterization**

Generally, 0.4 g $NaBH_4$ (96%, Sinopharm) was dissolved in deionized water (40 ml) at room temperature, and adding NaOH (97%, Aladdin) solution subsequently to regulate pH (12−14). Dissolving 0.8 g $SbCl_3$ (99%, Aladdin) in ethylene glycol solution (40 ml) while stirring vigorously until the solution is liquid. Then the $NaBH_4$ solution was gently added to the $SbCl_3$ solution, and placed the mixed solution for 2 h at 60℃ to allow the uninterrupted outgrowth of Sb. At last, centrifugally collected the powder with deionized water and absolute ethanol by a couple of times, and dried 5h in a drying oven at 80 °C for a preoxidation process of the as−obtained Sb powder. Later, kept the prepared Sb nanoparticles at 100, 200 and 300 °C in air about 3 h to obtain the oxidation of Sb, marked as $Sb/Sb_2O_3$-100, $Sb/Sb_2O_3$-200, $Sb/Sb_2O_3$-300, respectively, and the as−obtained Sb powder before annealing was marked as BA-Sb. To compare, the Sb nanoparticles was synthesized according to our previous reports [38, 39].

The XRD results were acquired from an X−ray diffractometer (RigakuD/MAX−2500, λ=1.54178 Å, Cu−Kα line). The Figure 8e was obtained by testing the electrode material coated on a copper foil. In order to avoid the interference of copper foil, the peak of copper foil is removed here. A field emission scanning electron microscope JEOL JEM−7100F (Japan) as well as TESCAN MIRA LMS (CZ) were used for SEM and EDX tests. Transmission electron microscope (TEM) images, high−resolution TEM (HRTEM) images were procured by a TMP field−emission transmission electron microscope (Tecnai G2 F20 S−TWIN). A LabRAM ARAMIS Raman spectrometer with the excitation wavelength of 633 nm was used for Raman spectra analysis. The BET results were tested by Quantachrome Autosorb IQ3, America. The XPS results were acquired from Thermo Scientific K−Alpha, America.

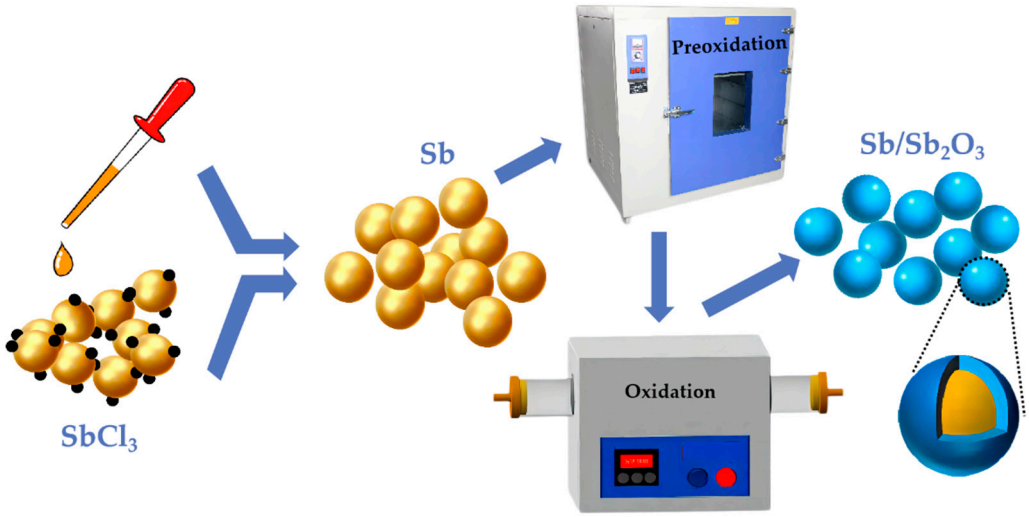


**Figure S1.** The schematically preparation process of $Sb/Sb_2O_3$ nanoparticles.

**Electrochemical performance mensuration**

The electrochemical performance of $Sb/Sb_2O_3$ as the active anode material for SIBs was measured in assembling coin cells (CR2032). At first, the anode electrode was composed of the prepared materials, acetylene black (50g, 99%, Shanghai sj–htech Co. Ltd.) and carboxymethyl cellulose (CMC) (99%, BYT–3000–180717, Shanghai sj–htech Co. Ltd.) with the weight ratio of 8:1:1. Then milled the components in agate mortar with deionized water to obtaining the viscous muld, and spread the muld on a clean copper foil. Put the treated copper foil into a vacuum drying oven for 8 h at 60 °C. Then using the punching machine to stamping the working electrode into discs with diameters of 12 mm, the mass loading of active material ($Sb/Sb_2O_3$) was in a range of 1.0−1.2 mg. Assembling the coin cells with these discs in an Ar–filled glovebox (Mikrouna). Choosing Na disk as the opposite electrode, glass microfibers (Whatman GF/F) as the diaphragm, and 1 M $NaClO_4$ in blended with propylene carbonate (PC) solution which added 3% fluoroethylenecarbonate (FEC) (Na114–1–210804–100mL, Shanghai sj–htech Co. Ltd.) as the electrolyte solution. The voltage window of galvanostatic charge–discharge test was 0.01–2 V within the LAND CT2001A test facility. The CV curves (at the scan rate of 0.1 mV $s^{-1}$) and the EIS curves (0.01 Hz–$1.0 \times 10^5$ Hz) were measured by the electrochemical work–station (CHI–660E).

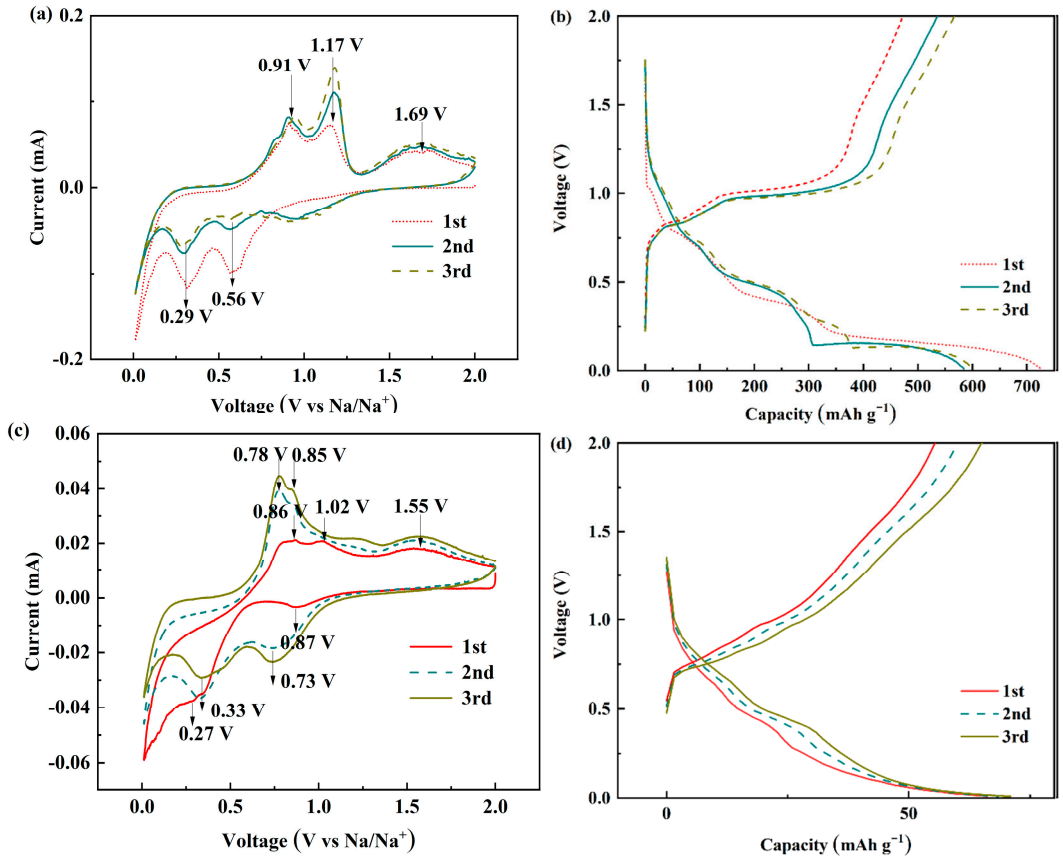


**Figure S2.** (**a**, **c**) CV curves of Sb/$Sb_2O_3$-100 and Sb/$Sb_2O_3$-300 over 0.01–2.0 V at 0.1 mV $s^{-1}$, (**b**, **d**) discharge/charge curves of Sb/$Sb_2O_3$-100 and Sb/$Sb_2O_3$-300 in the initial three cycles at 0.1 A $g^{-1}$.

**Table S1.** Parameters used in the model [32–34]

| Name | Description | Core | Shell |
|---|---|---|---|
| $C_{max}$ (mol $m^{-3}$) | maximum concentration | $1.65\times10^{5}$ | $1.65\times10^{5}$ |
| $C_0$ (mol $m^{-3}$) | initial concentration | 0 | 0 |
| $D_0$ ($m^2$ $s^{-1}$) | diffusion coefficient | $5.2\times10^{-13}$ | $1.4\times10^{-14}$ |
| R (m) | inner diameter/ external diameter | 1.5–3.2($\times10^{-8}$) | 3–7($\times10^{-8}$) |
| $v$ | poisson ratio | 0.28 | 0.23 |
| $E$ (Pa) | Young modulus | $2.37\times10^{10}$ | $3.14\times10^{10}$ |
| Ω ($m^3$ $mol^{-1}$) | partial molar volume | $3.497\times10^{-6}$ | $3.26\times10^{-6}$ |
| T (K) | temperature | 298 | 298 |