Supporting Information

Understanding the mechanism of enhanced cycling stability in Sn-Sb composite Na-ion battery anodes: operando alloying and diffusion barriers

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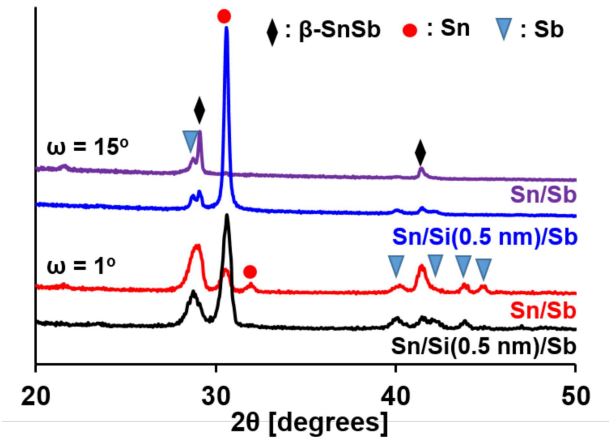

Figure S1. XRD patterns of the Sn/Si(0.5 nm)/Sb trilayer and Sn/Sb bilayer measured at ω = 1° and ω = 15°.

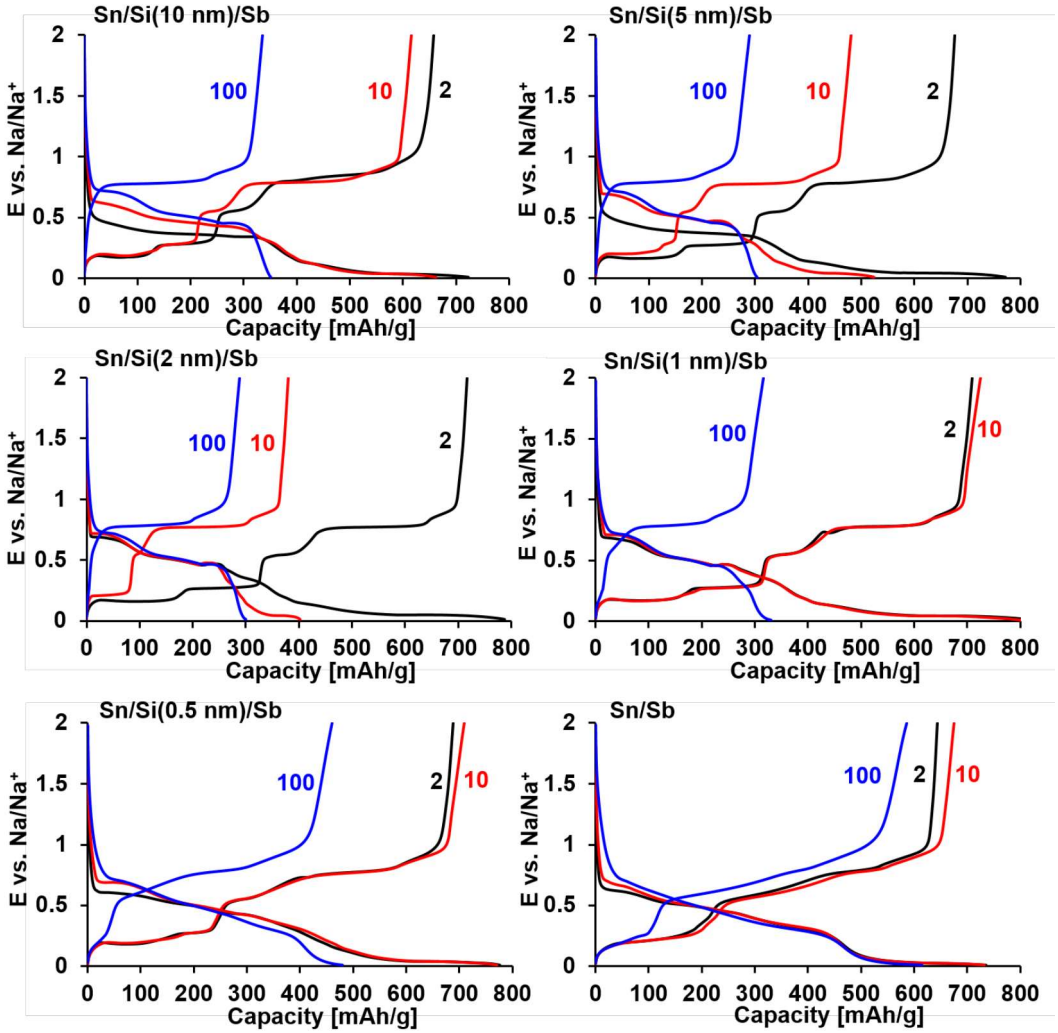

Figure S2. Voltage profiles for the cycles depicted in Figure 5.

Table S1. Breakdown of the theoretical maximum capacity and expansion contributions of each layer in Sn/Si(x nm)/Sb trilayers.

Layer	Thickness (nm)	wt. %	Maximum capacity contribution (mAh/g)	Maximum expansion (nm)
Sb	45-50	45.9-47.5	303-314	132-146
Sn	45-50	50.6-52.4	429-444	191-211
Si	0.5-10	0.17-3.6	1.6-34	0.8-14.4

The wt.% calculated for each layer in Table S1 is based on a density of 6.62, 7.30 and 2.32 g/cm^3 for Sb, Sn and Si, respectively. The maximum capacities were assumed to be 660 (Na_3Sb), 847 ($Na_{15}Sn_4$) and 954 (NaSi) mAh/g in the same order. The expansion at maximum sodiation is 293% for Sb,[1] 425% for Sn,[2] and 144% for Si.[3]

Table S2. Theoretical and measured maximum capacities as a function of Sb thickness in Sb(x nm)/Sn(100-x nm) bilayers.

Sb thickness (nm)	Theoretical capacity (mAh/g)	Measured capacity (mAh/g)
65	730	717
50	758	727
35	786	788
25	804	782
15	824	821
5	838	812
0	847	727

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(3) Witte, J.; Schnering, H. G.; Klemm, W. Das Verhalten der Alkalimetalle zu Halbmetallen. XI. Die Kristallstruktur von NaSi und NaGe. *Z. Für Anorg. Allg. Chem.* **1964**, *327*, 260–273.