Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supplemental information: Mechanical properties of Si/C composite electrode during lithiation

We prepared CMC/SBR-based Si/C composite electrode (SL-450A, 10% silicon content), maintaining consistency with the graphite electrode in terms of mass ratio, preparation process, and research methodology. The particle size distributions and porosity of active materials used in electrode preparation are presented in Table. S1. Samples of Si/C composite electrodes at various lithiation states were successfully obtained by fabricating 3032-type button cells. The stress-strain curves and mechanical properties of Si/C composite electrodes at different SOCs are obtained through uniaxial tensile experiments, with the results presented in Fig. S1.

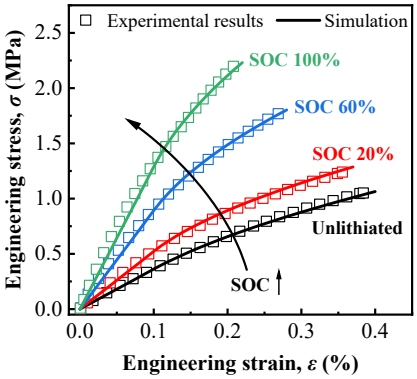

Fig. S1. Engineering stress-strain curves of Si/C composite electrode at different SOCs (Scattering points: experimental results; Curves: simulation).

Based on the stress-strain curves of Si/C composite electrodes at different SOCs, we derived the correction factor f with the expression given as $f = 1.185 \times \bar{c} + 5.012$. The strength parameters k and hardening index n are 20 MPa and 0.5, respectively. These results were utilized to fit the parameter K in the plastic hardening during lithiation. There is a linear relationship between the strength parameter K and $\bar{c}$, with the expression given as $K = 10 \times \bar{c} + 20\,(\mathrm{MPa})$. To simulate the elastic-plastic deformation of Si/C composite electrodes at different SOCs, quasi-static tensile simulations were performed using COMSOL software on rectangular films with dimensions of 25 mm × 5 mm. In terms of checking the prediction accuracy of the proposed model, the simulated uniaxial tensile mechanical behaviours of Si/C composite electrodes at various SOCs are compared with corresponding experimental results. As seen in Fig. S1, the model successfully captures the mechanical response of Si/C composite electrodes during lithiation. The result indicates that the proposed phenomenological model has a broad range of applications.

Table. S1. Active particle size distribution and porosity of active materials

Index	Graphite (S360-L2-H)	Si/C (SL-450A)
D10 (μm)	6.5	4.6
D50 (μm)	15.1	12.1
D90 (μm)	27.6	26.3
Porosity (SOC 0%)	41.83%	40.6%
Porosity (SOC 100%)	25.62%	26.05%