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Lithiation-Assisted Strengthening Effect and Reactive Flow in Bulk and Nano-Confined Sulfur Cathodes of Lithium-Sulfur Batteries
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— Sulfur (S) serves as a promising cathode material in Li-ion batteries owing to its abundance on earth, low cost and high theoretical specific capacity ˜1670 mAhg-1, which is 3-5 times higher than that of current commercial Li-ion batteries. Nowadays, the most popular strategies of using S cathode are based on producing nanostructured carbon matrices (i.e. hollow carbon nanospheres and nanofibers) to sustain S cathode loading. However, the possible stress evolution and mechanical degradation of the confined S cathode in those carbon matrices have never been explored before. In addition, the associated structural and conductivity changes of the confined S cathode during the lithiation/delithiation process plays a significant role in the battery performance. With the above in mind, here we conduct reactive molecular dynamics simulations to investigate the microstructural and stress evolution of the confined S cathode during lithiation/delithiation process. Simulation results indicate an unusual stress relaxation state in Li_xS compounds at lower Li concentrations ($x > 0.7$). The strength of corresponding Li-S compounds also increases with respect to the Li concentration.

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