



Mechanics-based optimization of yolk-shell carbon-coated silicon nanoparticle as electrode materials for high-capacity lithium ion battery



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ARTICLE INFO

Article history:

Received 8 March 2016

Accepted 21 July 2016

Keywords:

Anode

In situ TEM

Fracture mechanics

Optimal design

ABSTRACT

Yolk-shell carbon-coated silicon nanoparticles (Si@void@C NPs) have been demonstrated to have a great promise in solving the problem of significant volume change of silicon-based anode materials during lithiation and delithiation cycling. However, our *in situ* lithiation experiments show that Si@void@C NPs may still subject to fracture upon lithiation, depending on their characteristic structural features such as the size of Si yolk, the thickness of carbon shell, and the interspace between the yolk and shell. Given the size of Si yolk, to ensure structural integrity of Si@void@C NPs during lithiation and delithiation, thicker carbon shell and larger yolk-shell interspace are preferred. On the other hand, from the perspective of attaining higher effective capacity, thinner carbon shell and smaller yolk-shell interspace are favored. To find the optimal structural design which yields the maximum capacity and meanwhile ensure the integrity of Si@void@C NPs during lithiation, mechanics-based theoretical modeling is carried out. A diagram for structural optimizations is obtained, by which the optimized Si@void@C NPs are synthesized and found to have improved capacity and capacity retention compared to the unoptimized ones. The results of this paper provide a guideline for the design of Si@void@C NPs as anode materials for high-capacity lithium ion battery.

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1. Introduction

Lithium ion battery (LIB), as an energy storage and supply unit, has been widely used in various devices from household electrics to industrial facilities [1]. In order to achieve high capacity and long lifespan, a variety of electrode materials of LIB have been applied. The prevailing carbon-based anode materials, despite of long cycle life, exhibit low capacity (372 mA h g^{-1}) [2,3]. In contrast, silicon (Si) anode materials possess high capacity (4200 mA h g^{-1}) but suffer from fracture and pulverization due to the large volume change ($\sim 400\%$) during lithiation and delithiation cycling, leading to poor cycle life [4]. Although reducing the Si anode materials to nanoscale has been demonstrated to have improved performance, solid electrolyte interface (SEI) would form on their surfaces whose repeated fracture and

thickening, upon cyclic lithiation and delithiation, consume the Si and electrolyte, leading to the degradation of electrochemical performance of the battery [5–7]. To solve this problem, carbon-coated Si nanowires and nanoparticles (NPs) have been developed and found able to improve the cycle life of pure nano Si materials [8–10]. However, because of the adding of carbon whose specific capacity is much lower compared to that of Si, the effective capacity of the anode material decreases. Structural optimization was applied to maximize the capacity on the condition that the structural integrity got ensured [11,12]. More recently, yolk-shell carbon-coated Si (Si@void@C) NPs, which incorporate spare space between the Si yolk and carbon shell, have been developed, exhibiting much better electrochemical performance [13–20]. The improved cycling performance is mainly due to the interspace that can accommodate the lithiation-induced expansion of the Si yolk and thereby mitigates the stress and deformation of the carbon shell. As a consequence, the SEI formed on the surface of carbon shell will not fracture during the electrochemical cycling. Nevertheless, in literature the capacities of the LIBs using Si@void@C NPs as anode materials exhibit

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a wide spectrum ranging from a few hundreds to more than 2000 mA h g^{-1} , implying much room in optimizing the Si@void@C NPs. For example, it is still unclear how much space should be spared between the Si yolk and carbon shell and how thick the carbon shell should be so as to achieve the highest capacity and simultaneously maintain the structural integrity of

Si@void@C NPs during lithiation and delithiation cycling. The objective of this paper is to find such optimal design of Si@void@C NP, at least in principle, for high-capacity LIBs.

The remaining of this paper proceeds as follows. First, we carry out *in situ* lithiation on individual Si@void@C NPs with different sizes and shell thicknesses to deduce the factors

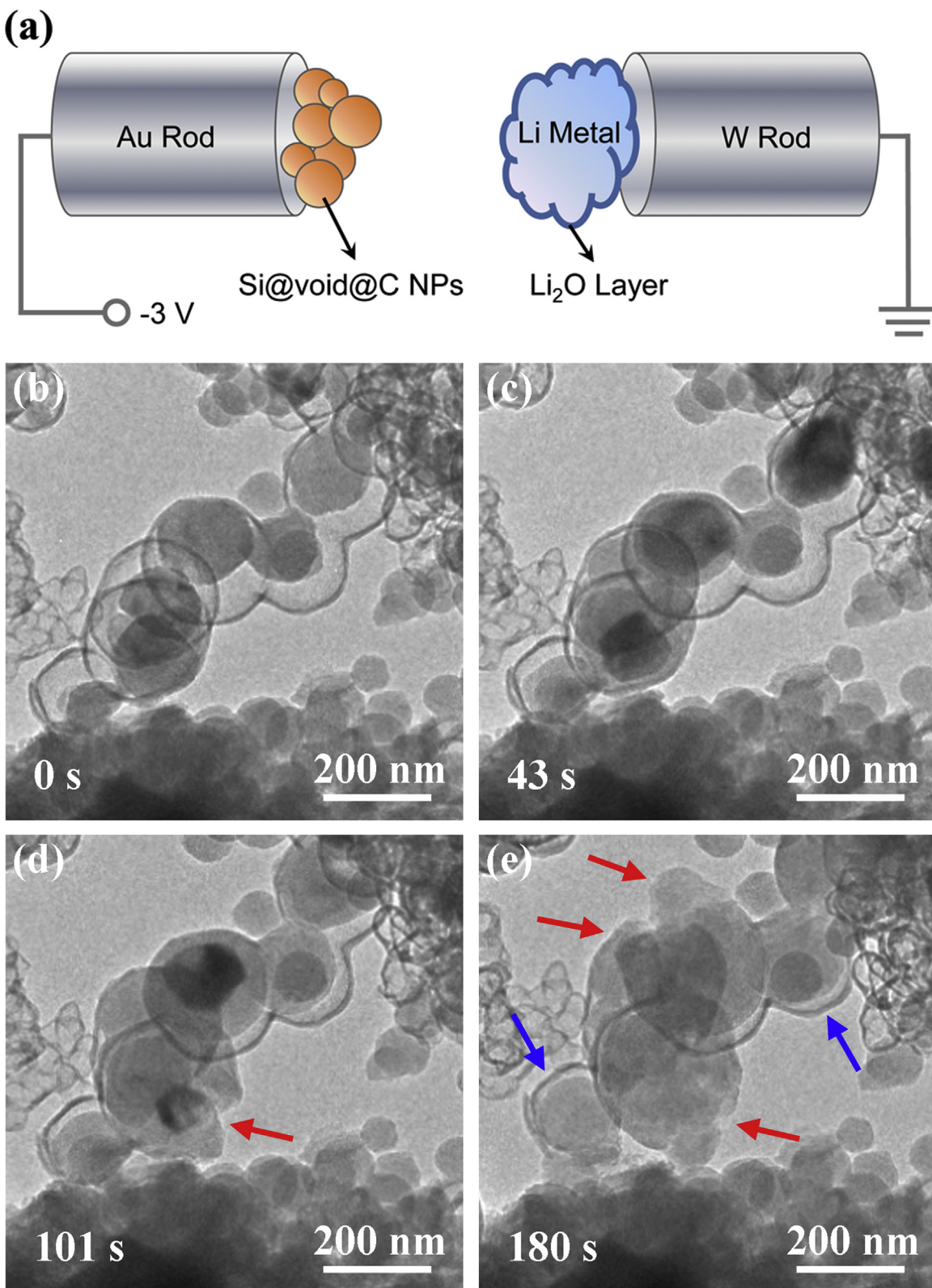


Fig. 1. (a) Schematic of the setup for *in situ* lithiation. (b–e) Snapshots of the lithiation process for the Si@void@C NPs.

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