Rigid TiO_{2-x} Coating on Mesoporous Hollow Si Spheres with High Structure Stability for High Performance Lithium-Ion Battery

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High–energy–density Li–ion batteries with long–cycle and high–rate performances are in great demand for the development of electric vehicles [1, 2]. Silicon is regarded as a potential alternative to commercially used graphite due to its high theoretical capacity (4200 $mAh \cdot g^{-1}$). Unfortunately, particle pulverization resulting from the tremendous volume change during operation and inherently low electrical conductivity seriously limit its electrochemical performance and large-scale application.

In this work, we developed a facile approach for the fabrication of mesoporous hollow silicon spheres@TiO_{2-x} (MHSi@TiO_{2-x}) nanocomposite through the magnesiothermic reduction of hollow silica nanospheres, in situ tetrabutyltitanate hydrolysis on the MHSi surface, and sequent calcination in inert atmosphere.

Results and Discussion

As shown in Figure 1, the mesoporous hollow structure can be clearly observed, and the mesoporous Si is surrounded by a uniform TiO_{2-x} coating layer. At a current density of 2 $A \cdot g^{-1}$, MHSi@TiO_{2-x} delivers a high reversible specific capacity of 1303.1 $mAh \cdot g^{-1}$, and 84.5% capacity retention after 500 cycles.

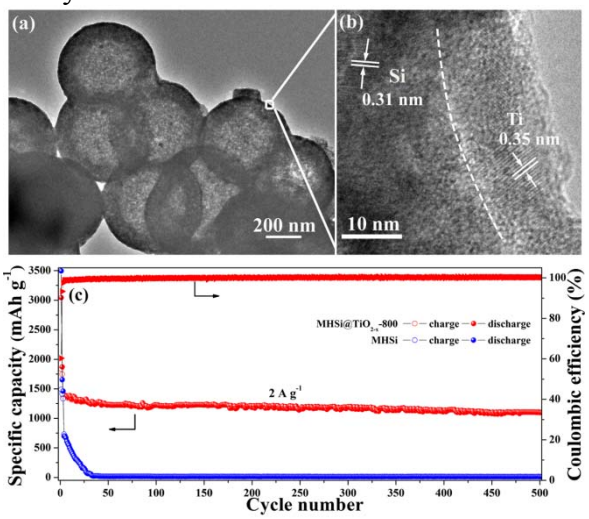

Figure 1. (a,b) HRTEM images of the MHSi@TiO_{2-x} composite, (c) Cyclic performance of MHSi and MHSi@TiO_{2-x} at 2 $A \cdot g^{-1}$.

Conclusion

In summary, an interface-engineered Si-based anode with a mechanically and electrically robust structure has been synthesized via a facile method. The conductive TiO_{2-x} shell not only enhances the transport kinetics of electron and Li^+, but also provides a rigid structure with high mechanical stability to confine the outward expansion of Si, maintaining the structural integrity and a stable SEI. The mesoporous hollow structure provides enough void space for expansion of Si, effectively buffering large volume change. As a result, MHSi@TiO_{2-x} anode yields excellent cycling stability and superior rate capability.

References:

[1] Y. Jin, S. Li, A. Kushima, Y. Cui, et al. Energy Environ. Sci. 10 (2017) 580-592.
[2] M. Gu, Y. He, J. Zheng, C. Wang, Nano Energy 17 (2015) 366–383.