LI-ION REACTION MECHANISMS IN SILICON NANOTUBES

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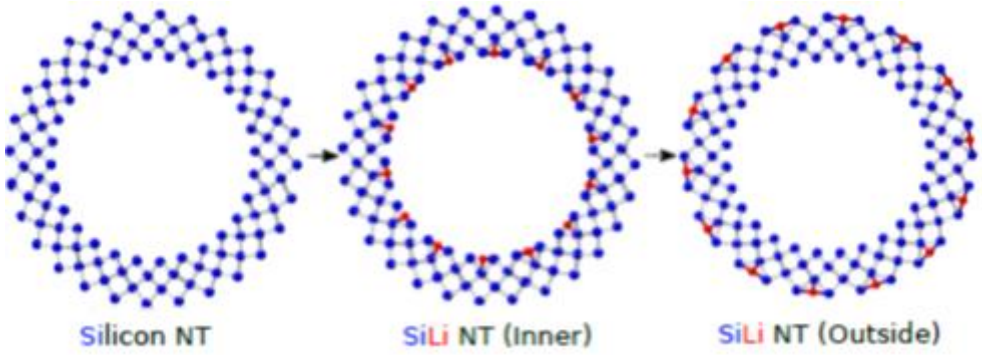
Rechargeable lithium-ion batteries are considered to be the most promising energy storage due to their long cycle life and high specific capacity [1]. However, existing lithium-ion batteries use graphite as anode material and this is not efficient enough to reach market level to be employed in vehicles. There are still some challenges to develop more in anode material to enhance their performance to meet the requirements for efficient energy storage [2]. Silicon has been regarded as one of the most promising candidate to replace graphite anode material due to its excellent merits in high theoretical electrochemical capacity. It is safe to use in high-power applications due to its low discharge potential [3]. However, the commercial application of silicon in the battery is still not progressed due to severe mechanical damage because of volume expansion and contraction of Si electrodes during cycling operation. This could cause pulverisation and loss of capacity [4]. An effective way to solve this problem is the employment of nanostructures, which are capable of minimising the volume change due to small size and available surrounding free space [5].

The aim of this study is to understand how the use of silicon nanotubes can improve the performance of Li-ion batteries. For this purpose we are using a combination of experimental techniques and atomistic simulations to determine the atomic processes involved in the insertion and extraction mechanisms of lithium ions in the silicon nanotubes. It is found that the strain energy in the tubes favour Li-ion insertion in the outer part of the tubes, as opposed from the inside of the tubes, which is in agreement with experimental observations. Experimentally, these findings are combined with electrochemical studies of silicon nanotubes, using a number of various electronic conducting binders and Li-ion salts.



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