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Simulation Studies on Stress Generation and Volume Expansion Due to Electrochemical Lithium Insertion in a Silicon Nanowire

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Abstract

Silicon electrode is presently being pursued as a potential negative electrode for lithium-ion batteries owing to its high gravimetric (mAh/g) and volumetric capacity (mAh/L) compared to the existing state of the art graphite electrode. There are several key challenges which have to be overcome for efficient performance of Si as a negative electrode. One of the critical challenges is to minimize particle fracture due to internal stresses, developed during lithiation/delithiation of Si electrode. Recent experimental studies have demonstrated the use of nano size Si electrodes which minimizes insertion induced stresses due to facile strain relaxation. In this talk, the results from a transient two-dimensional numerical model which simulates the lithium insertion process in a cylindrical Si NW anchored to a current collector substrate will be presented. The model predicts volume expansion/shape changes; stresses developed due to chemical and elastic strains in the material, and the voltage curves as a function of lithium content in Si under galvanostatic operation. The effect of operating and design parameters on the stress evolution and voltage curves will also be discussed.

Reference

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3. John Christensen and John Newman, J. Solid State Electrochem.10, 293 (2006)
4. Rajeswari Chandrasekaran, Alexandre Magasinski, Gleb Yushin, and Thomas F. Fuller, J. Electrochem. Soc., 157, A1139 (2010)

Figures used in the abstract

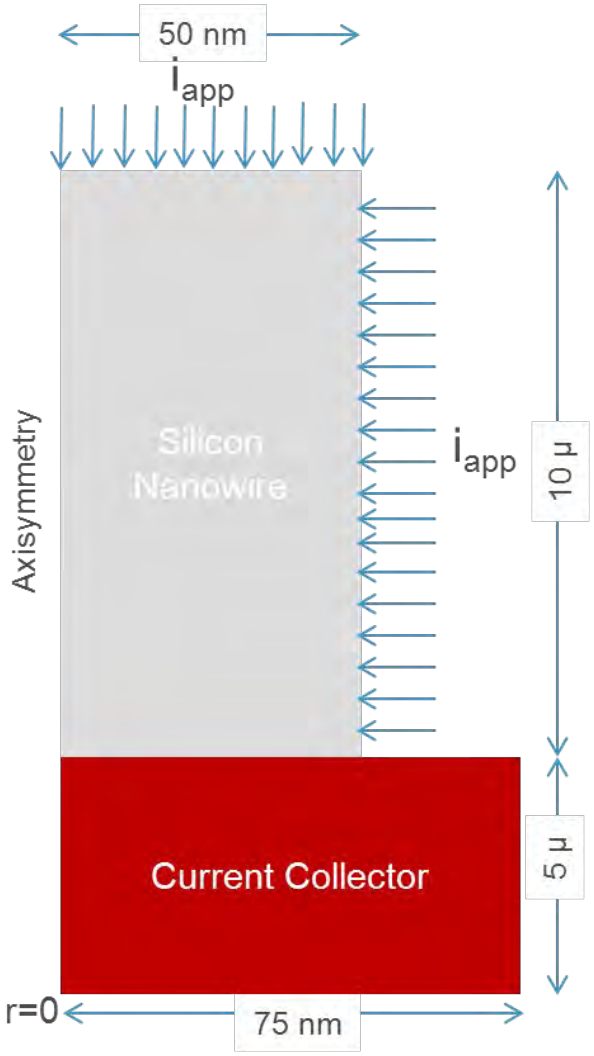

Figure 1: Model geometry which contains a cylindrical Si NW anchored on to a current collector substrate

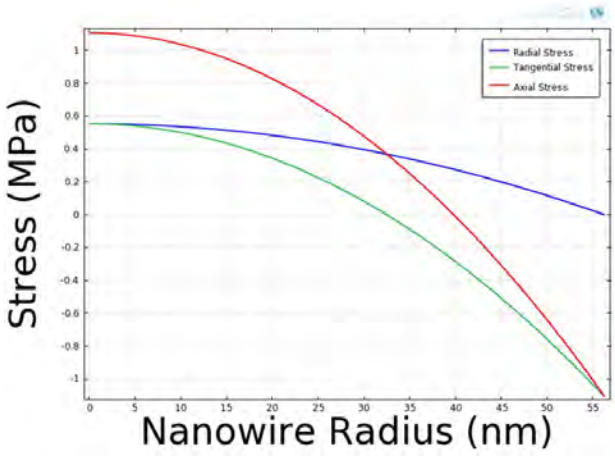

Figure 2: Plot showing the radial, tangential and axial stresses developed across the radius of the Si NW (halfway along the height of the Si NW). The stress profiles correspond to galvanostatic discharge of Si NW at 500s