Mechanical properties of silicon nanowire anodes at different states of charge

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ABSTRACT

Silicon is considered to be a promising anode material for lithium-ion batteries with very high energy densities. During lithiation, silicon anodes form different Li–Si phases and store up to 3.75 lithium ions per silicon atom. Associated with this high capacity is a volume change of roughly 300% and large mechanical stresses that may affect the electrochemical processes. The stresses that actually form strongly depend on the mechanical properties of the lithium silicides and the mechanical processes that occur inside the anode material during operation. So far, only very limited knowledge exists on the mechanics of lithiated silicon. In order to gain insight into the mechanics of silicon anodes, mechanical experiments on individual silicon nanowires were carried out. Nanoscale tensile experiments were performed in situ inside an SEM on crystalline silicon nanowires in the pristine state as well as after lithiation and subsequent delithiation. In the delithiated state the wires are amorphous and exhibit dramatically reduced strength and modulus when compared with crystalline silicon. Experiments on fully lithiated silicon wires also show a reduced Young’s modulus. In these wires plastic yielding takes place at stresses ~1 GPa. For lower stresses, a time dependent deformation process was identified. In the Li3.75Si wires, the strain rate depends linearly on the stress so that the observations can be described as viscous flow with a viscosity of $6 \times 10^{13}$ Pas. This mechanical behavior is similar to that of glass heated to around 500°C. The findings suggests that besides plasticity also this time dependent deformation mechanism may need to be considered to correctly describe the processes of lithiation and delithiation of silicon.