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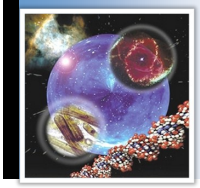
Fracture of Crystalline Silicone Nonopillars during Electrochemical Lithium Insertion

Understanding the insertion of lithium into silicon electrodes for high capacity lithium-ion batteries is likely to have benefits for mobile energy storage, for both electronics and transportation. Silicon nanostruc-tures have proven to be attractive candi-dates for elec-trodes because they provide less constraint on the vol-ume changes that occur and more resistance to fracture during lithium insertion. But still, facture can oc-cur even in silicon nanostructures. Here, we consider the fracture of Si nanopillars dur-ing lithiation and find surprising results. We find that fracture is initiated at the surfac-es of the nanopillars and not in the interior, as had been predicted by analyses based on diffusion-induced stresses. In situ transmission electron micros-copy observations of initially crystalline Si nanoparti-cles shows that lithiation occurs by the growth of an amorphous lithiated shell, subjected to tension, at the expense of a crystalline Si core, subjected to compres-sion. We also show that the expansion of the nanopillars is highly anisotropic and that the fracture locations are also anisotropic. In addition, we find a critical fracture diameter of about 300nm that appears to depend on the electrochemi-cal reaction rate. Modeling the stress evo-lution in Si nanopillars during lithiation pro-vides a way to understand and control these failure processes. Also, we show that ini-tially amorphous Si nanopillars are much more resistant to failure because the stresses at the surface are largely compressive in this situation compared to tension in the case of initially crystalline nanopillars.



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