Materials Science and Engineering
Distinguished Scholar Lecture

FEATURING

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Fracture of Silicon Nanopillars during Electrochemical Lithium Insertion
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ABSTRACT
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 nanostructures have proven to be attractive candidates for electrodes because they provide less constraint on the volume changes that occur and more resistance to fracture during lithium insertion. But still, fracture can occur even in nanostructured silicon. Here, we consider the fracture of Si nanopillars during lithiation and find surprising results. We find that fracture is initiated at the surfaces of the crystalline nanopillars and not in the interior, as had been predicted by analyses based on diffusion-induced stresses. In situ transmission electron microscopy observations of initially crystalline Si nanoparticles 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 compression. 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 for initially crystalline nanopillars of about 300nm that appears to depend on the electrochemical reaction rate. Modeling the stress evolution in Si nanopillars during lithiation provides a way to understand and control these failure processes. Also, we show that initially amorphous Si nanopillars are much more resistant to failure, having much larger critical fracture diameters, because the stresses at the surface are compressive in this situation compared to tension in the case of initially crystalline nanopillars. For sufficiently big amorphous Si nanopillars, cracking is initiated in the interior, as expected from the diffusion-induced stresses. It is hoped that these studies will be useful in the design of silicon electrodes for advanced battery systems.

BIOSKETCH
Professor Nix obtained his B.S. degree in Metallurgical Engineering from San Jose State College, and his M.S. and Ph.D. degrees in Metallurgical Engineering and Materials Science, respectively, from Stanford University. He joined the faculty at Stanford in 1963 and was appointed Professor in 1972. He was named the Lee Otterson Professor of Engineering at Stanford University in 1989 and served as Chairman of the Department of Materials Science and Engineering from 1991 to 1996. He became Professor Emeritus in 2003. In 2001 he was awarded an Honorary Doctor of Engineering Degree by the Colorado School of Mines and in 2007 an honorary degree of Doctor of Engineering by the University of Illinois. He received an honorary degree of Doctor of Science from Northwestern University in 2012.

In 1966 he participated in Ford Foundation's "Residence in Engineering Practice " program as Assistant to the Director of Technology at the Satellite Division of Union Carbide Corporation. From 1968 to 1970 Professor Nix was Director of Stanford's Center for Materials Research. Professor Nix is engaged in research on the mechanical properties of solids. He is principally concerned with the relation between structure and mechanical properties of materials in both thin film and bulk form and is also engaged in research on the mechanical properties of materials for lithium-ion batteries. He is co-author of 450 publications in these and related fields and he has trained 77 Ph.D. students in these subjects in his years at Stanford. Professor Nix teaches courses on dislocation theory and mechanical properties of materials. He is co-author of "The Principles of Engineering Materials", published in 1973 by Prentice-Hall, Incorporated.