Stress and strain in silicon electrode models

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Graphite is currently the standard active material used in commercial lithium-ion battery negative electrodes. Materials such as silicon are attractive alternatives to graphite because they have significantly higher capacities for inserted lithium;higher lithium capacities will enable production of batteries with higher energy densities.

Unfortunately, large volume changes due to insertion and removal of lithium produce mechanical stresses in host materials. These, in turn, exert stress on the surrounding material in porous electrodes. These stresses can cause mechanical damage, leading to electrical isolation of active material and capacity fade.

This project asks where mechanical damage is likely to occur, and under which situations damage might be avoided. Detailed stress measurements at the scale of the active material particles would be very difficult to obtain, and a lack of ordered structure makes it impractical to create detailed mathematical descriptions of porous electrodes. For these reasons, simple numerical models of adjacent binder and active material regions were studied to gain basic insight about mechanical processes that might occur in a far more complicated porous electrode.

A new general-purpose simulation package was developed and used to calculate stresses and strains throughout two-dimensional model systems. These calculations include shear stresses at interfaces between binder and active material regions, which do not arise in spherically-symmetric systems. Comparison of computed stresses and strains with material properties suggest if and where material damage is likely to occur in the various model systems, as well as possible approaches for limiting mechanical damage.