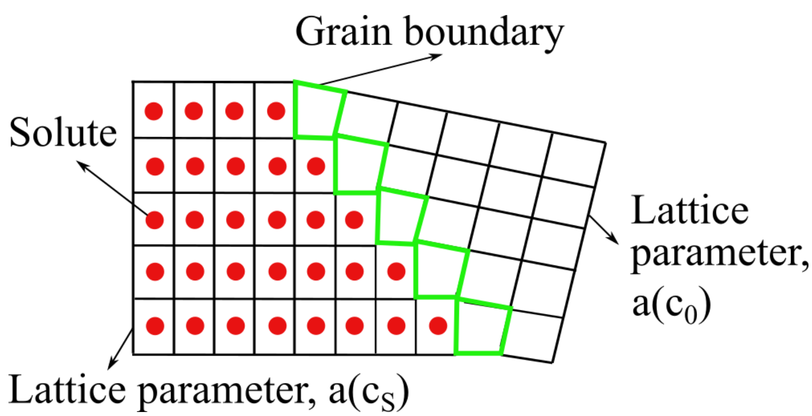
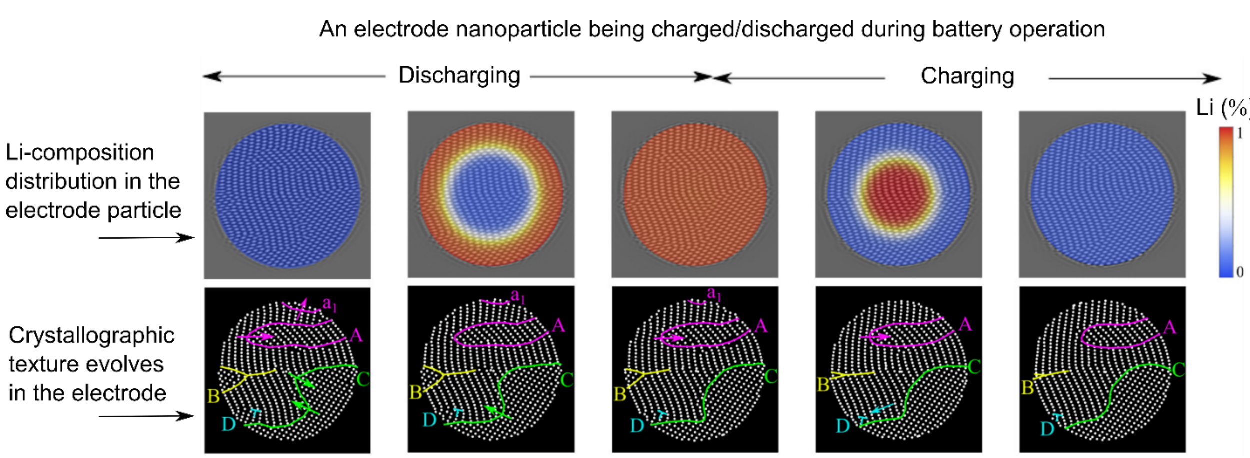
Every few years, we notice a drop in our phone's battery capacity. Eventually, we need to replace these batteries, which is not only expensive but also depletes earth's reserves of rare elements. There are several causes for battery fade, such as depletion of active ions, discharge rate and mechanical degration of battery materials. In our recent paper, we demonstrate that repeatedly charging/discharging a battery is another reason, which makes electrodes brittle and prone to failure.

Li diffuses into interstitial lattice sites during battery operation



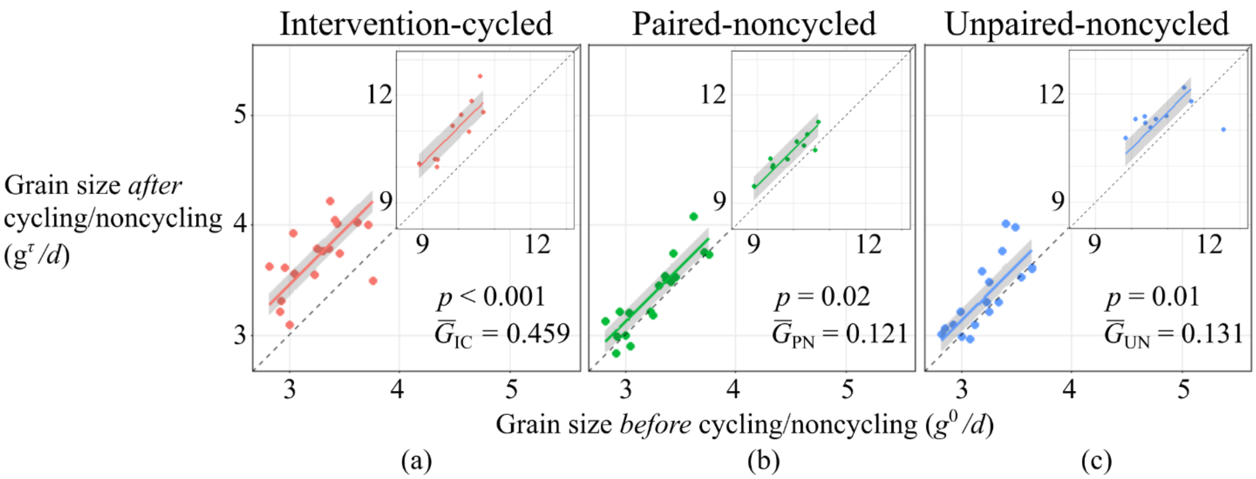
During a charge/discharge cycle, Li-diffuses through an electrode's interstitial lattice sites and can induce substantial volume changes. This creates a gradient in lattice parameters as a function of Li-concentration, which produces stresses at the proximity of a grain boundary. We hypothesize that these stresses induce grain boundary movement that affect an electrode's mechanical strength.

Multiscale modeling of electrode microstructures



We test our hypothesis by computing grain growth in sixty $FePO_4$ electrodes in two parallel studies. In the first study, we electrochemically cycle the electrode and calculate Li-diffusion induced grain growth. In the second study, we do not cycle the electrode and calculate curvature-drive grain growth.

Li diffusion induces grain growth in electrodes



We find a statistically significant grain growth in the cycled electrodes, and negligible grain growth in the noncycled electrodes. These results suggest that Li-diffusion is an additional process that increases mean grain size in electrodes.

Overall, we find that repeatedly charging/discharging a battery influences the crystallographic texture of its materials, which makes them brittle and prone to failure.

Reference

- Balakrishna, A. R., Chiang, Y. M., & Carter, W. C. (2019). Phase-field model for diffusion-induced grain boundary migration: An application to battery electrodes. Physical Review Materials, 3(6), 065404.