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**Shape and volume changes in Lithiated Silicon anodes for batteries** EKIN CUBUK, WEI WANG, EFTHIMIOS KAXIRAS, Harvard University — Silicon is one of the most promising materials for use as an anode for Lithium-ion batteries due to its capacity to hold a large number of Li atoms (up to 4.4 Li per Si atom). One of the biggest challenges in using Silicon as anode material is mechanical failures due to large volume expansion during the lithiation process. Recently detailed experiments have been reported on the dependence of volume change on the crystal orientation, especially for nano-scale structures. We investigate the microscopic mechanisms for shape changes during lithiation of Si by comparing the reaction mechanisms of Li atoms on different surfaces of crystalline Si using first-principles calculations.

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