

Simulations of the First Charge of Nanobatteries: Silicon Anodes

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ABSTRACT

In order to understand the mechanics and chemistry of silicon electrodes and to prevent undesirable effects such as the cracking of the anode, research have been performed using nanoscale approaches to a fully nanobattery. We studied both, the graphite and the silicon nanocrystal anodes, performing ab initio calculations and classical molecular dynamics atomistic simulations. In this effort in progress we are focusing on the mechanical properties, such as swelling, alloying mechanism, and amorphization of the anode material during the first charging cycle and also the electrical properties such as polarization and current. The nanobattery includes LiCoO_2 cathode; the electrolyte solution contains ethylene carbonate, as well as hexafluorophosphate and Li-ions. In these preliminary models, a solid electrolyte interface (SEI) is not included yet. An external electric field is applied to emulate the charging process causing the migration of the Li-ions from the cathode, diffusing through the electrolyte to finally get into the anode. We immediately observe during charging (i.e., when an external electric field is applied) of the nanobattery, the Si anode changes gradually into a LiSi alloy at temperatures below 360 K. We obtained the drift velocity of the Li-ions during the amorphization of the silicon nanocrystal as the original volume of the anode increases. For the graphite anode, the full lithiated state is achieved when the initial structure C changes into LiC_6 , storing the Li-ion between the layers of the graphite, thus we were able to compare energy, temperature, and electrical properties such as current, resistance, current density, conductivity and resistivity. Our model can be used to study the mechanisms taking place in the electrolyte, cathode, and especially for new materials for the anode.