

ANALYSIS OF A LI-ION NANOBATTERY WITH GRAPHITE ANODE USING MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Initially the loading of a Li-ion nanobattery with a graphite anode and lithium hexafluorophosphate (LiPF₆) salt dissolved in ethylene carbonate (CO₃C₂H₄) as the electrolyte solution was carried out with molecular dynamics simulations. By applying external electrical fields simulating voltage sources, the charging was accomplished. Li-ion behavior that travels from cathode to anode through concentration electrolyte alternatives is studied. To study the mechanism behind the diffusion of the Li-ions through the SEI, a solid electrolyte interphase (SEI) layer was also added to the model. As the battery is loaded, the depletion of Li atoms in the cathode and their anode accumulation follow a linear rise in the solvent's polarizability until a saturation point is reached after which the battery charging stops.

Key words: Li-ion nanobattery, cathode, anode.

INTRODUCTION

Li-ion batteries, particularly in-home electronics, are one of the most common electrochemical technologies. Li has one of the Periodic Table's lowest ionization energies, 5.39 eV^{1,2} and is therefore the easiest to ionize among the first 10 atoms; Li-ion's atomic radii can be as low as 0.73 Å, almost half the neutral atom radii. Despite the high level of sophistication required in Li-ion batteries [1] for their right charging and discharge cycles, the need for unique circuitry for protection and safety and its elevated price compared to other options, such as Na, K, Ni or Pb, among others, Li is still very common owing to its low self-discharge when not in use and its elevated gravimetric and volumetric energy densities, resulting in light weight batteries.

METHODOLOGY

The module: Classical molecular dynamics (MD) simulations are conducted using the Large Scale Atomic Molecular Massively Parallel Simulator (LAMMPS)[2], [3] program to calculate

worldwide characteristics and to predict the conduct of the electrolyte solution and anode of a nanobattery. The original simulation box size is 166.6 between 27.0 and 58.2 Å³, identified in the three directions with periodic boundary conditions (PBCs). There are 21 LiPF₆ dissolved in 310 EC molecules as part of the electrolyte solution, resulting in an electrolyte solution of 1.15 molar (1.15 M).

The Force Fields: The electrolyte solution is based on LiPF₆ salt, which in ethylene carbonate (EC) dissolves into Li⁺ ions and PF₆⁻ counter ions. The intramolecular interactions are derived from the force field of CFF93; however, specific parameters, bonds, angles, dihedrals and inappropriate dihedrals for EC and LiPF₆ are derived from the use of the Gaussian-09[4], [5] program with the cc-pVT basis set and ZB3PW91 function. The intermolecular force field parameters for Lennard-Jones (LJ) interactions between the atoms of EC, Li in LiCoO₂, PF₆, and graphene are taken from UFF47 using their average rules for pairs of different types of atoms ; however, some of the specific pair interactions have been adjusted rather than using the usual average quantities to prevent EC or PF₆ from entering the threshold where there is no presence of an electric field.

RESULT

Equilibration and Settings

The battery is balanced at 293 K for 10 ns; the energy stabilizes at -5,66±0,03 Gcal / mol after the first 3 ns of balance. Atomic motions can be described as changes during this final equilibrium, so the nanobattery shows no radical change in composition or phase.

First Charge of the Nanobattery

An electrical field E is implemented to simulate the charging of the battery after the balance at 293 K. The electrons start to move in different directions due to the field due to which the layer of graphite consist of 45 Li atoms. The number of Li-ions entering the anode gradually increases during charging. With that the ionic current can be obtained under steady conditions. Simulations are conducted for up to 400 ps and allowed to move through the electrolyte and reach the anode in computationally practical times.

CONCLUSION

In addition to the end of loading owing to the depletion of Li in the cathode, the saturation of Li in the anode, or the increase of temperature to excessive values that could alter the stage or characteristics of the electrolyte, a very significant extra factor to consider is the time to achieve peak polarizability in the electrolyte environment after which battery charging is not practical and it takes place long before any of the other three scenarios are reached. On the SEI, or even directly on the anode of a fresh battery, the dipole moment can have a powerful impact on Li-plating. Thus, excessive polarization during charging can improve Li-dendrites' local formation, which can cause the battery to shorten the circuit.

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