Numerical modeling of dendrite growth in a lithium air battery system

Authors: Jinwang Tan, Emily Ryan
Affiliation: Department of Mechanical Engineering, Boston University
Address: 110 Cummington Mall, Boston, MA 02215

Lithium air (Li-air) batteries are a promising advance battery technology that are being considered for portable and automotive applications. The practical energy densities of Li-air batteries could rival those of gasoline due to the high reactivity of Li and the use of atmospheric air as a reactant. However, before a high energy, reliable Li-air battery can be achieved several design and operational challenges need to be overcome. Dendrite formation is one challenge that causes performance and safety issues in current lithium batteries. Dendrites form on the surface of the lithium anode after multiple charge/discharge cycles. The formation of dendrites changes the local transport properties and the scale of the critical physics of the anode. It can also lead to increased Joule heating in the anode and eventual breakage of the dendrites, which may cause short circuits. The study of dendrite growth can provide insight into the physics that cause the growth and possible methods for suppressing dendrite growth, which could lead to the development of a more reliable Li-air battery.

In this research a simplified physical model of dendrite growth is developed to simulate growth during the charging process. The dendrite growth model is based on previous work by other groups who theoretically and experimentally investigated dendrite growth in similar systems.[1-3] In the current model the growth of dendrites are determined by the local charge density, overpotential, ion concentration and ion diffusivity in electrolyte. The growth of side branches are modeled in relation to the growth of the main dendrite via a power law relation. Our model shows that the dendrite growth is sensitive to ion diffusivity in electrolyte and the velocity of the dendrite growth decreases significantly when ion diffusivity increases. Furthermore, the growth velocity approaches linear time dependence under high ion diffusivity. The current density also plays an important role in dendrite growth, which means increasing current density will accelerate the growth of dendrites.

References

1. Bockris, J.L.B.a.J.O.M., *The electrolytic growth of dendrites from ionic solutions.* JECS, 1962.
2. Chazalviel, J.N., *Electrochemical Aspects of the Generation of Ramified Metallic Electrodeposits.* Physical Review A, 1990. **42**(12): p. 7355-7367.
3. Monroe, C. and J. Newman, *Dendrite growth in lithium/polymer systems - A propagation model for liquid electrolytes under galvanostatic conditions.* Journal of the Electrochemical Society, 2003. **150**(10).