Computational modeling of Silicon anodes: the role of mechanics on the electrochemical performance

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Abstract:

In an attempt to address future needs for energy storage and transportation, researches have proposed the use of Silicon anodes in Li-ion batteries. Such Silicon based anodes have the potential to achieve about 10 times the capacity of current generation graphite anodes. However, the intercalation of such a large amount of Lithium into the silicon induces very large deformations of the anode leading to volume changes of approximately 300%. These large volumetric changes, accompanied by plastic deformation, can have significant deleterious effects on the mechanical and electrochemical performance of the anode.

In this talk, I will present a thermodynamically consistent constitutive framework to model the coupled problem of diffusion of Lithium into a deforming host. Using a robust finite-element implementation, the theory is calibrated to experiments available in the literature. Further, using the calibrated theory we model a Silicon anode which is composed of double-walled hollow nano tubes, a promising design, which has been experimentally realized in the literature. We will show that our simulation tool is capable of predicting the electrochemical performance of the anode and can be used to elucidate the role of mechanical deformation on the performance of the anode.

About the Speaker:

Claudio Di Leo is a PhD candidate in the Department of Mechanical Engineering at the Massachusetts Institute of Technology where his research focuses on modeling the coupled multi-physics behavior of energy storage materials. He received his M.S. and B.S. from MIT where he worked on computational modeling of hydrogen storage in metals and experimental efforts in enhancing shape memory polymers. Recently, he was the recipient of the best graduate student paper award at the SES annual meeting for work on modeling phase-separating cathode materials

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