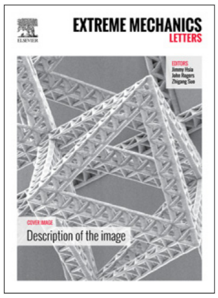

A large deformation elastic-viscoplastic model for lithium

Sooraj Narayan, Lallit Anand

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A large deformation elastic-viscoplastic model for lithium

Sooraj Narayan and Lallit Anand*
Department of Mechanical Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139, USA

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Abstract

An essential ingredient in modeling the response of lithium in an all-solid-state lithium battery in which a lithium metal anode is paired with a non-flammable inorganic solid electrolyte (SE), is a constitutive model for the large deformation elastic-viscoplastic response of lithium. Wang and Cheng (2017) have recently published indentation load-versus-depth data from their microindentation experiments conducted in an argon-filled glove box to study the viscoplastic behavior of lithium at room temperature. In this paper we report on a large deformation isotropic elastic-viscoplastic theory for modeling the response of lithium. We have implemented the theory as a user-material-subroutine in a finite element program, and the material parameters for the theory have been calibrated using the data from the microindentation experiments of Wang and Cheng. To exhibit the utility of our finite element simulation capability, we show results from two representative numerical simulations of relevance to modeling the mechanical interaction between a lithium anode and a SE: (a) flattening of an asperity on the surface of lithium when it is mechanically impressed by a flat ceramic SE; and (b) intrusion of lithium into a cavity on the surface of SE, when the SE is mechanically impressed into lithium with a flat surface.

Keywords: lithum; microindentation; viscoplasticity; finite element

1 Introduction

There is substantial ongoing world-wide research on all-solid-state lithium batteries, which have the potential to substantially improve the energy density, safety, and performance of battery systems for electric vehicles. The key components of such a battery are: (i) a pure metallic Li-anode, which has a high theoretical gravimetric capacity of 3860 mAh/g, relative to a current generation graphitic anode, which has a capacity of only 372 mAh/g; and (ii) a non-flammable solid-electrolyte (SE) with high ionic conductivity $\gtrsim 10^{-3}\,\mathrm{S\,cm^{-1}}$, which also acts as the separator between the anode and the cathode. Non-flammable inorganic solid electrolytes, when paired with lithium metal anodes, could result in high energy density, yet safe rechargeable lithium batteries. Indeed, the successful incorporation of metallic lithium anodes in batteries is widely considered one of the major challenges in the design, manufacture, and operation of the next generation Li-battery based energy storage devices (Albertus et al., 2018).

A Li/SE interface is always present in any kind of solid-state battery, regardless of the cathode, and ensuring stable lithium plating and stripping at a Li/SE interface is of major importance for the realization of high-performance solid-state lithium batteries. A major obstacle in the operation of solid-state batteries — which must be overcome — is the redistribution of lithium and its intrusion into defects at the surface of the SE, and the subsequent growth of lithium through the electrolyte under charge-discharge cycles to cause a short-circuit.

*Tel.: +1-617-253-1635; E-mail address: anand@mit.edu