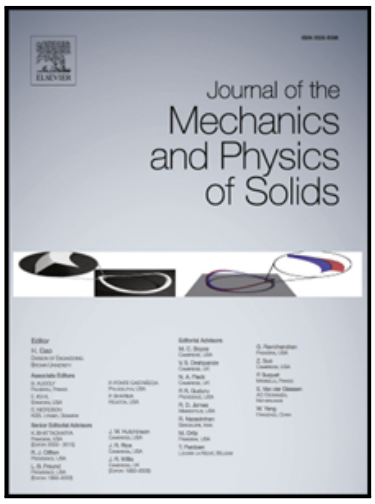

Corrosive fracture of electrodes in Li-ion batteries

Rong Xu , Kejie Zhao

PII: S0022-5096(18)30549-0
DOI: https://doi.org/10.1016/j.jmps.2018.07.021
Reference: MPS 3400

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 27 June 2018
Revised date: 27 July 2018
Accepted date: 27 July 2018

Please cite this article as: Rong Xu , Kejie Zhao , Corrosive fracture of electrodes in Li-ion batteries, *Journal of the Mechanics and Physics of Solids* (2018), doi: https://doi.org/10.1016/j.jmps.2018.07.021

Corrosive fracture of electrodes in Li-ion batteries

Rong Xu, Kejie Zhao*

School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907, USA

ABSTRACT

Fracture in electrochemical systems is often corrosive in nature. In Li-ion batteries, Li reaction causes embrittlement of the host material and typically results in a decrease of fracture toughness of anodes when Li inserts and a reduction of fracture toughness of cathodes when Li extracts. The dynamics of crack growth depends on the chemomechanical load, kinetics of Li transport, and the Li embrittlement effect. We implement a theory of coupled diffusion, large deformation, and crack growth into finite element modeling and simulate the corrosive fracture of electrodes under concurrent mechanical and chemical load. We construct the phase diagram delineating the unstable, arrested, and delayed fracture zones. We examine in detail the competition between energy release rate and fracture resistance as crack grows during both Li insertion and extraction. The wait-and-go behavior in the delayed fracture zone relies on the chemomechanical load and the supply of Li to the crack tip. We apply the theory to model the intergranular fracture in $LiNi_xMn_yCo_zO_2$ (NMC) particles which is the major mechanical degradation of the cathode material. The structural decohesion is induced by the mismatch strain at the grain boundaries. The evolving interfacial strength at different states of charge and different cycle numbers measured by in-situ nanoindentation is implemented in the numerical simulation. We model the corrosive behavior of intergranular cracks in NMC upon Li cycles and compare the crack morphologies with experiments.

Keywords: Fracture, diffusion, corrosion, chemomechanics, Li-ion batteries.

*Corresponding author: kjzhao@purdue.edu (K. Zhao)