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Cohesive modeling of crack nucleation in a cylindrical electrode under axisymmetric diffusion induced stresses

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ABSTRACT

We have recently modeled crack nucleation in a 2D strip electrode as localization of a periodic array of cohesive zones subject to diffusion induced stresses in an initially crack-free thin strip under galvanostatic solute insertion and extraction. Here we generalize this model to crack nucleation in a cylindrical electrode under axisymmetric diffusion induced stresses, focusing on the effect of the cylindrical geometry on the crack nucleation condition. Similar to our previous findings for the 2D strip geometry, the present analysis identifies a critical electrode size, typically in the nanometer range, to avoid crack nucleation.

1. Introduction

The technological needs to develop damage resistant lithium-ion battery electrodes with very large stresses and volume changes during Li intercalation–deintercalation cycles are calling for studies on crack nucleation under diffusion induced stresses. In the past, numerous models have been developed to describe the insertion/extraction of Li in an electrode as diffusion of interstitial atoms in a host material (García et al., 2005; Christensen and Newman, 2006a,b; Zhang et al., 2007, 2008; Cheng and Verbrugge, 2008, 2009; Deshpande et al., 2010a,b; Haftbaradaran et al., 2010, 2011; Yang, 2010), a subclass of problems more broadly referred to as the diffusion induced stresses (DIS) (Prussin, 1961; Li, 1978; Yang, 2005). In comparison, relatively few studies have explicitly considered crack nucleation under DIS. Huggins and Nix (2000) considered a bilayer plate with the top layer subjected to a swelling transformation strain and the bottom layer containing a crack. The Huggins–Nix model has been extended to the case of non-uniform distribution of DIS to predict relationships between charging rate, size and fracture toughness of an electrode particle for preventing growth of pre-existing cracks (Woodford et al., 2010; Zhao et al., 2010, 2011). In contrast, we have developed a cohesive model of crack nucleation in a strip electrode under galvanostatic charge and discharge (Bhandakkar and Gao, 2010). Compared to the Huggins–Nix model and its extensions (Huggins and Nix, 2000; Woodford et al., 2010; Zhao et al., 2010, 2011) which used Griffith's criterion to predict a critical condition for crack growth, the Bhandakkar–Gao model considers spontaneous localization of a periodic array of cohesive zones during dynamic evolution of DIS in an initially crack-free electrode.

Recent years have seen the development of various forms of cylindrical electrodes such as nanorods, nanopillars and nanowires, with improved performance and cycle life compared to planar and spherical electrode geometries (Taberna et al., 2006; Chan et al., 2008). The exact mechanism behind the superior mechanical response of cylindrical electrodes is unresolved and is being actively pursued (e.g. Huang et al., 2010). In the present paper, we extend the 2D Bhandakkar–Gao model to localization of an array of cohesive zones in a cylindrical electrode under axisymmetric diffusion induced stress as the maximum DIS exceeds the cohesive strength of the material (Fig. 1). Such localized deformation is thought to be initially reversible, and crack nucleation is assumed to occur when the maximum surface separation within the cohesive zone reaches a critical value.

2. Diffusion induced stress in a cylindrical electrode

Fig. 1 shows a cylindrical electrode with diameter $2r_c$ subject to insertion and extraction of an interstitial species such as Li. The electrode material is taken to be an isotropic linear elastic solid and the deformation is assumed quasi-static. Following an analogy

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