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Effect of diffusion-induced bending on diffusion-induced stress near the end faces of an elastic hollow cylinder

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ABSTRACT

Diffusion-induced stress plays an important role in determining structural integrity of mechanical structures used in lithium-ion batteries and microelectromechanical devices. Incorporating the diffusion-induced bending in the analysis of the diffusion-induced stress in an elastic hollow cylinder, analytical forms of the diffusion-induced resultant axial stress and hoop stress have been formulated for the traction-free condition and the built-in condition at the end faces of the cylinder. Using these results, the evolution of the diffusion-induced stress at the end faces of a hollow, elastic electrode due to the insertion of lithium is discussed under the potentiostatic operation. The end faces of the electrode experience compressive hoop stress through the thickness in contrast to the stress state in the hollow cylinder far away from the end faces. The magnitude of the resultant hoop stress decreases with increasing the diffusion time for the traction-free end faces; it increases with increasing the diffusion time near the inner surface for the built-in end faces.

1. Introduction

Lithium ion batteries (LIBs) have the potential applications in hybrid electric vehicles and electric vehicles. In the heart of LIBs are the intercalation and de-intercalation processes during electrochemical charging and discharging, which involve the diffusive motion of lithium atoms in the host electrodes of LIBs. The intercalation and de-intercalation of lithium atoms in the host electrodes of LIBs can cause volumertric change and local stress which can lead to structural degradation of the host electrodes. For example, the intercalation of Li-atoms between graphite sheets can introduce 10% of volumetric expansion in active graphite, which is the most common material used in the negative electrode of LIBs (Dah, 1991). Compared to graphite, silicon can incorporate 4.4 lithium atoms per silicon ($Li_{22}Si_5$), which gives a specific discharge capacity of 4200 mAh/g (Wen and Huggins, 1981). One of the important issues involving the use of Si-based materials in LIBs is the large change of specific volume (up to about 400%) during the intercalation and de-intercalation of lithium into silicon (Beaulieu et al., 2003). To accommodate the local stress introduced by the intercalation and de-intercalation of lithium atoms in the host electrodes, various low-dimensional structures, including nanoparticles (Han et al., 2011; Jiang et al., 2011; Martin et al., 2011), nanowires (Chan et al., 2008; Xu et al., 2011), and nanotubes (Chen et al., 2005; Martin et al., 2011) have been used as nanostructural electrodes, which have relatively long cyclic life as compared to the corresponding bulk materials.

The structural degradation and damage due to the intercalation and de-intercalation of lithium atoms in the host electrodes is associated with the stress evolution controlled by the diffusion of Li-atoms and chemical reaction in the host electrodes. The phenomenon of diffusion-induced stress was first studied by Prussin (1961). Li (1978) analyzed the evolution of diffusion-induced stress in elastic materials of simple geometries. Lee and co-workers (Lee et al., 2000; Wang et al., 2002) studied the evolution of chemical stresses in a hollow cylinder. Yang and Li (2003) analyzed the bending of an elastic beam induced by the diffusion of solute atoms. Considering the interaction between diffusion and chemical stresses, Yang (2005) derived the diffusion equation taking account of the effect of stress-induced diffusion, and established an analytical relation between hydrostatic stress and the concentration of solute atoms and obtained a general relation among the surface concentration of solute atoms, normal stress and surface deformation of a solid. Zang and Zhao (2012) introduced a diffusion and curvature dependent surface elastic model in the stress analysis of anode in lithium ion battery. Recently, Yang (2010a) incorporated the volumetric change due to local solid reaction into the theory of diffusion-induced stress in solid and derived a general relation among the concentration of solute atoms, local reaction product, and mechanical stress.

To improve the structural integrity of LIBs, various studies have been performed on the diffusion-induced stress due to the intercalation and de-intercalation of lithium atoms in the host electrodes (Christensen and Newman, 2006; Gao and Zhou, 2011; Kalnaus

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Nomenclature

C	the concentration of the diffusing component
D	the flexural rigidity
E	Young's modulus
M	the bending moment induced by the diffusion
u_r	radial component of the displacement vector
w	transverse deflection of the hollow cylinder
ν	Poisson's ratio
ε_{ij}	the components of strain tensor
σ_{ij}	the components of stress tensor
Ω	the coefficient of the volume expansion per mole of solute atoms
Subscripts i and j	r, θ, and z

et al., 2011; Woodford et al., 2010; Yang, 2010b; Zhang et al., 2007). However, these studies have been using ideal geometries, such as sphere and cylinder of infinite length. There is little study on the geometric effect on the evolution of the diffusion-induced stress in a solid.

Understanding the stress evolution in the host electrodes of LIBs is critical for controlling the structural durability of LIBs. The purpose of this work is to analyze the effect of diffusion-induced bending on the diffusion-induced stress at the end faces of an elastic hollow cylinder, which mimics the intercalation and de-intercalation of lithium atoms in nanotubes. The analysis is focused on establishing analytical formulation of the diffusion-induced stress at the end faces of the hollow cylinder with the traction-free condition and the built-in condition. The stress evolution at the end faces of an elastic hollow electrode under the potentiostatic operation is also discussed.

2. Diffusion-induced stress in an elastic hollow cylinder

Consider the diffusion-induced stress in an elastic hollow cylinder with inner radius of r_i and outer radius r_o. The hollow cylinder is at an externally "stress-free" state, while it experiences self-stressing due to the diffusion of solute atoms in radial direction. For the present purpose, only linear elastic deformation is considered. The constitutive relations describing the diffusion-induced deformation in a cylindrical coordinate (r, θ, z) are

$$\varepsilon_{ij} = \frac{1}{E}[(1+\nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij}] + \frac{C\Omega}{3}\delta_{ij} \tag{1}$$

where ε_{ij} are the components of strain tensor, σ_{ij} are the components of stress tensor, Ω is the coefficient of the volume expansion per mole of solute atoms, and C is the concentration (moles/m^3) of the diffusing component, E and ν are Young's modulus and Poisson's ratio of the material, respectively. The subscripts i and j can be r, θ, and z.

Assume that the concentration of solute atoms in the hollow cylinder is only a function of r and the length of the hollow cylinder is much larger than the outer radius. In general, the characteristic time for elastic deformation of solids is much smaller than that for diffusive motion of atoms. Static equilibrium can prevail at all times. For the deformation in the hollow cylinder far away from the cylinder ends, the stress state in the hollow cylinder can be approximated as the plane strain. Due to symmetrical characteristics of the problem, there is only one non-zero displacement component, u_r, of the displacement vector. The strain components in terms of the displacement component, u_r, are

$$\varepsilon_{rr} = \frac{du_r}{dr} \text{ and } \varepsilon_{\theta\theta} = \frac{u_r}{r} \tag{2}$$

The differential equation for the radial displacement, u_r, is

$$\frac{d}{dr}\left(\frac{1}{r}\frac{dru_r}{dr}\right) = \frac{\Omega}{3}\frac{1+\nu}{1-\nu}\frac{dC}{dr} \tag{3}$$

Without the action of external loading and body force, the boundary conditions of the hollow cylinder far away from the cylinder ends are

$$\sigma_{rr}(r_i, t) = \sigma_{rr}(r_o, t) = 0 \tag{4}$$

Using the boundary conditions of (4), the stress distribution in the hollow cylinder far away from the cylinder ends then can be found as (Lee et al., 2000)

$$\sigma_{rr} = \frac{E\Omega}{3(1-\nu)}\frac{1}{r^2}\left(\frac{r^2 - r_i^2}{r_o^2 - r_i^2}\int_{r_i}^{r_o} Crdr - \int_{r_i}^{r} Crdr\right) \tag{5}$$

$$\sigma_{\theta\theta} = \frac{E\Omega}{3(1-\nu)}\frac{1}{r^2}\left(\frac{r^2 + r_i^2}{r_o^2 - r_i^2}\int_{r_i}^{r_o} Crdr + \int_{r_i}^{r} Crdr - Cr^2\right) \tag{6}$$

and the displacement component, u_r, as

$$u_r = \frac{\Omega(1+\nu)}{3r(1-\nu)}\left(\int_{r_i}^{r} Crdr + \frac{(1-2\nu)r^2 + r_i^2}{r_o^2 - r_i^2}\int_{r_i}^{r_o} Crdr\right) - \nu\varepsilon_z r \tag{7}$$

2.1. Effect of traction-free ends

If an elastic hollow cylinder with traction-free ends is subjected to a uniform change of concentration, no chemical stresses will be produced. With the presence of the concentration gradient in the radial direction, there is no bending at points at a large distance from the free ends, and the stresses can be calculated from Eqs. (5) and (6). Near the ends there will be some bending, which will create chemical stresses in the elastic hollow cylinder. The resultant diffusion-induced stresses consist of the stresses given in (5) and (6) and the bending-induced stresses, and are necessary to satisfy the stress-free conditions.

For an elastic hollow cylinder with traction-free ends, the resultant diffusion-induced stresses must vanish at the ends, and ε_{zz} is a constant in the axis of the hollow cylinder. Thus, there are

$$\sigma_{zz}^r = \sigma_{rz}^r = \sigma_{\theta z}^r = 0 \tag{8}$$

at the end faces of the hollow cylinder. Here, the superscript r represents the resultant stress in the hollow cylinder. From Eq. (7) and the relationship between the displacement components and the strain components, there are $\sigma_{rz}^r = \sigma_{\theta z}^r = 0$. An additional condition is required to have $\sigma_{zz}^r = 0$.

It is very difficult if not impossible to obtain the exact solution of the stress distribution near the end faces of the hollow cylinder. An approximation can be made to have

$$\sigma_{zz}^r = \langle\sigma_{zz}\rangle + \sigma_{zz} \tag{9}$$

with the uniform stress $\langle\sigma_{zz}\rangle$ being determined by the following condition

$$2\pi\int_{r_i}^{r_o}\sigma_{zz}^r rdr = \pi(r_o^2 - r_i^2)\langle\sigma_{zz}\rangle + 2\pi\int_{r_i}^{r_o}\sigma_{zz}rdr = 0 \tag{10}$$

From the constitutive equations of (1), there is

$$\sigma_{zz} = \nu(\sigma_{rr} + \sigma_{\theta\theta}) + E\left(\varepsilon_{zz} - \frac{C\Omega}{3}\right) = \frac{\nu E\Omega}{3(1-\nu)} \times \left(\frac{2}{r_o^2 - r_i^2}\int_{r_i}^{r_o} Crdr - C\right) + E\left(\varepsilon_{zz} - \frac{C\Omega}{3}\right) \tag{11}$$