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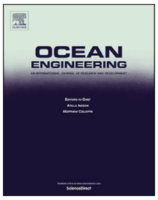

Peridynamic modelling of fracture in marine lithium-ion batteries

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A B S T R A C T

Lithium ion battery is one of the most promising energy storage equipment due to its high energy density and long life cycle, and it has various applications in marine industry. Coupled diffusive-mechanical process during cycling has significant influence on ion diffusion and stress evolution. This may cause large deformation of electrodes which is the main reason of crack nucleation and propagation. As a consequence, this will have a negative effect on battery performance in terms of electrical capacity and thermal stability, and can cause failure of the battery. Hence, crack propagation and stress evolution during lithiation of the electrode plate is under investigation in this study. Peridynamics, as a new computational technique, is utilized for this purpose and various validation and demonstration cases were considered to demonstrate the capability of the developed framework.

1. Introduction

Energy conservation and emission control are the most concerning issues in marine industry. According to Marpol Annes VI regulations, the emission of nitrogen oxide in 2016 should be restricted below 80% of that in 2000 and the emission of sulfur oxide should be reduced around 90% in 2020 by comparing with the amount in 2012 (Herdzik, 2011). As one of the solutions in emission reduction, the hybrid marine electric propulsion system has become popular in marine transportation. In this system, energy transmission and thrust operation can be directly controlled by electric power plant such as a battery. Therefore, fuel consumption and waste gas emission can be significantly reduced (Chen et al., 2010). Marine batteries are under extensive investigation to optimise the battery performance and reduce the cost.

Based on battery applications, marine batteries can be categorised into starting batteries and deep cycle batteries (Dougherty et al., 2002). Starting batteries are designed to start the marine engine with relatively high power output in a short period. Hence, starting batteries are usually composed of series of thin electrode plates to increase electrochemical reaction surface. However, a thin electrode does not have strong stiffness for harsh operating environment and does not support deep cycle charging. On the other hand, although deep-cycle batteries (or reserve batteries) may not have strong energy output, they have relatively large capacity which can discharge for a long time (Dougherty et al., 2002; Rosenkranz, 2003). Therefore, deep-cycle marine batteries are always made to provide additional power for the auxiliary system and the propulsion system.

Based on battery chemistry, marine batteries can be classified in several types such as lead-acid batteries, lithium-ion batteries and sulfur batteries. Detailed advantages and disadvantages of different battery types are given in Table 1. Apart from cost, marine lithium ion battery is one of the most promising power storage systems due to its high energy density, low self-discharge and long life cycle (Rosenkranz, 2003; Chung et al., 2002). Lithium ion batteries have various applications in marine environment such as in tugboats, ice-breakers and cruise ships.

The performance of lithium ion battery mainly depends on the material properties of electrodes and electrolyte. The selection of electrode material is based on the operating environment of the lithium-ion batteries. For the cathode material, Cobalt compound and Nickel compound are highly electrically stable, but they are toxic and are not very thermally stable. On the other hand, manganese compound has relatively high electrical capacity and high thermal stability, but it has low cycle performance (Daniel, 2008). Alternatively, silicon and its compound have become attractive as battery electrode material due to its high theoretical capacity (3600–4200Ahg^{-1}), excellent cycling stability and low price (Grantab and Shenoy, 2012; Chan et al., 2008). However, silicon based electrodes experience large volumetric expansion (around 300%–400%) during lithiation (Grantab and Shenoy, 2012; Chan et al., 2008; Liu et al., 2012). Frequent cycling causes stress misdistribution which may lead to crack initiation and growth. This will have a negative influence on battery performance. Once a crack forms, stress will concentrate at the crack tips. It has been observed that large amount of lithium ions rush into the crack tip region and increase the ion concentration of this region. As a result, the crack tip region has relatively larger

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Table 1
Comparison of battery technologies (Zhou et al., 2013).

Battery type	Advantages	Disadvantages
Lead-acid	Low cost Low self-discharge (2-5% per month)	Short life cycle (1200~1800 cycles) Life cycle affected by depth of charge Low energy density (about 40 Wh/kg)
Nickel-based	Can be fully charged (3000 cycles) High energy density (50-80 Mi/kg)	High cost, 10 times of lead acid battery High self-discharge (10% per month)
Lithium-ion	High energy density (80~190 Mi/kg) Very high efficiency (90~100%) Low self-discharge (1~3% per month)	Very high cost ($900-1300/kWh) Life cycle severely shorten by deep discharge Require special overcharge protection circuit
Sodium	High efficiency (85~92%)	Pre-heated in stand-by mode at 325°C
Sulphur (NaS)	High energy density(100 Wh/kg) No degradation of deep charge No self-discharge	
Flow battery	Independent energy and power ratings Long service life (10000 cycles) No degradation for deep charge Negligible self-discharge	Medium energy density (40~70 Wh/kg)

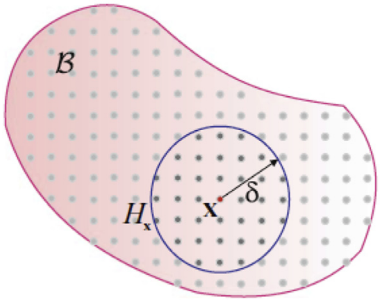

Fig. 1. Horizon of the material point x (Madenci and Oterkus, 2014).

expansion as compared to other parts and the stress reduces. Hence, lithium ion diffusion and stress distribution has a direct influence on each other. To represent this interaction accurately, full coupled numerical models are necessary. So far, finite element method (FEM) has been mainly used by using cohesive zone model (Grantab and Shenoy, 2012) and phase-field approach (Zuo and Zhao, 2015). As a new numerical technique, peridynamics (Silling, 2000) can be a suitable alternative for FEM based models and can eliminate certain numerical issues such as convergence, mesh dependency, etc. Therefore, in this study, peridynamics has been used to predict fracture propagation during the lithiation process for the first time in the literature.

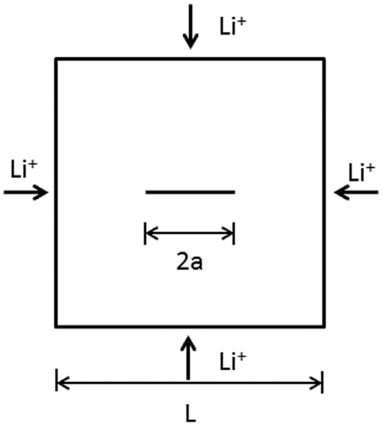

Fig. 2. Pre-cracked square shape electrode plate specimen (Zuo and Zhao, 2015).

Table 2
Parameters in numerical simulation.

E	Elastic constant of silicon	$80GPa$
ν	Poisson's ratio of silicon	0.22
Ω	partial molar volume	$8.5 \times 10^{-6} m^3 mol^{-1}$
M	molecular mobility	$500 m^2 J^{-1} s^{-1}$
k_B	Boltzmann constant	$1.38 \times 10^{-23} J{\cdot}K^{-1}$
T	absolute temperature	$300K$
N_A	Avogadro's constant	$6.02 \times 10^{23} mol^{-1}$
ε_c	threshold strain	0.04
$q_{\max}$	maximum concentration	$1.18 \times 10^4 molm^{-3}$

2. Coupled lithium diffusion and stress evolution on electrode plate

As mentioned earlier, silicon based electrodes can experience large volume expansion during the lithiation process. Frequent cycling may lead to crack initiation and growth. Once a crack emerges inside the electrode, stresses will concentrate at the crack tips. It has been observed that large amount of lithium ions quickly moves to the crack tip region and increase the ion concentration of this region. As a result, the crack tip region has relatively larger expansion by comparing with other parts and the stress reduces. This process can be expressed as (Zuo and Zhao, 2015):

$$\frac{\partial q}{\partial t} = Mk_BT\left(\frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2}\right) - \frac{Mq\Omega}{N_A}\left(\frac{\partial^2 \tilde{\sigma}}{\partial x^2} + \frac{\partial^2 \tilde{\sigma}}{\partial y^2}\right) - \frac{Mq\Omega}{N_A}\left(\frac{\partial q}{\partial x}\frac{\partial \tilde{\sigma}}{\partial x} + \frac{\partial q}{\partial y}\frac{\partial \tilde{\sigma}}{\partial y}\right) \tag{1}$$

where q represents the concentration of lithium ion and $\tilde{\sigma}$ is the hydrostatic stress which can be expressed for a two-dimensional case as (Malvern, 1969)

$$\tilde{\sigma} = \frac{1}{2}(\sigma_{11} + \sigma_{22}) \tag{2}$$

with σ_{11} and σ_{22} being diagonal terms of the Cauchy stress tensor. The stress distribution in classical continuum mechanics can be obtained by solving the equation of motion as:

$$\sigma_{ij,j} + b_i = \rho \ddot{u}_i \tag{3}$$

where b represents body load, ρ is the mass density and $\ddot{u}_i$ is the acceleration of a material point. The stress tensor, σ_{ij}, can be expressed in terms of strains as

$$\sigma_{ij} = \frac{E\nu}{(1+\nu)(1-2\nu)}\varepsilon_{ii}\delta_{ij} + \frac{E}{(1+\nu)}\varepsilon_{ij} - \frac{E\Omega}{2(1-\nu)}q\delta_{ij} \tag{4}$$

where ε_{ij} is the strain tensor, E and ν represents Elastic modulus and Poisson's ratio, respectively, Ω is the partial polar volume and δ_{ij} is the Kronecker delta. In Eq. (4) the last term represents the effect of lithium concentration on deformation field. Since the focus of this paper is predicting fracture, obtaining solution for Eqs. (1) and (3) is difficult since discontinuities occur as a result of crack existence and spatial derivatives at discontinuities are not defined. To analyse such cases, special treatments are necessary which may be cumbersome. Instead, these equations can be represented in a different form without using spatial derivatives,