A Numerical Study on the Heat Generation in $LiCoO_2$ Cathode Electrode by Using X-Ray Nano-CT Images

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Rechargeable lithium ion batteries (LIBs) have been considered as a promising power source for electric vehicles due to their high energy and power densities, high voltage and low self-discharge rate (1). However, significant thermal concerns still exist in a battery cell or a battery pack (1-3). For instance, overheating and uneven heating within each individual battery cell and across the entire battery pack during charge and discharge cycles can lead to fast battery degradation (4). Moreover, a local hotspot generated by uneven heating could trigger thermal runway, thus leading to the failure of a battery and safety issues (5). Therefore, fundamental understanding of the heat generation mechanisms inside LIBs during charge and discharge processes is necessary.

The thermal modeling of LIBs was pioneered by Newman and his coworkers and extended by many other researchers. To this end, the majority of the thermal models are based on the porous-electrode theory that assumes electrodes to be homogeneous and active materials particles to be spherical (6). Although the porous-electrode theory and simple active material structure models can be used to investigate LIB thermal effects with less time consumption of numerical simulation, the results cannot account for the non-uniform local heat generation and temperature distribution in LIBs. Because of the real complicated morphology of LIB electrodes (7), the interaction between electrode particles can cause non-uniform spatial distribution of the electrochemical field and heat generation. Therefore, the numerical approach with the details of electrode microstructure is desired for the study on the intricate local thermal effects in LIB electrodes.

In this work, we studied the heat generation in a real three dimensional (3D) microstructure of a $LiCoO_2$ cathode electrode during galvanostatic discharge processes. A $LiCoO_2$ cathode electrode of a LIB was scanned to obtain the microstructure using x-ray nano-CT technology (8). The previously developed 3D numerical framework (8) was extended to investigate the heat generation including the electronic and ionic resistive heat, the contact resistive heat, the reaction heat, the entropic heat and the heat of mixing during isothermal galvanostatic discharge processes. The results of heat generation rate at 1 C and 10 C discharge rates at 25˚C are shown in Fig. 1. The entropic heat plays a dominant role in the total heat generation at 1 C discharge rate. At 10 C discharge rate, the reaction heat and resistive heat start to count for a large fraction of the total heat generation. The heat of mixing is always much less than the other heat sources and can be neglected. Fig. 2 shows the distribution of ionic resistive heat in the electrolyte and the distribution of reaction heat at the interface between the electrolyte and the cathode particles. The results show that the heat generation is non-uniform and the magnitude of heat generation rate spans several orders in the inhomogeneous $LiCoO_2$ cathode electrode.

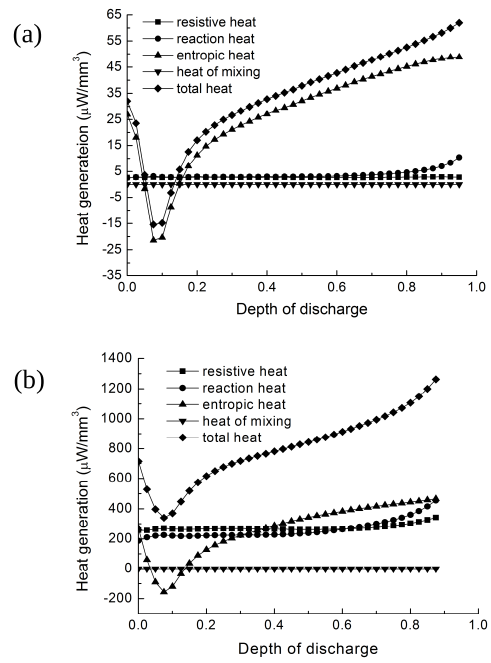

Fig. 1 Heat generation rate at 1C (a) and 10 C (b) discharge rate in the inhomogeneous electrode.

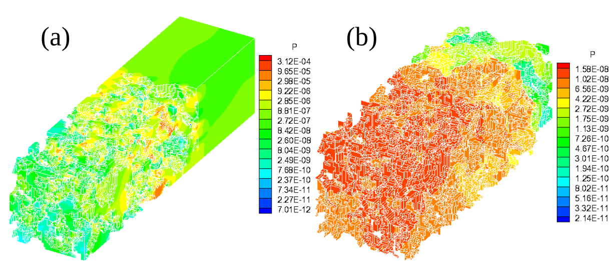

Fig. 2 (a) Distributions of the ionic resistive heat in the electrolyte and (b) the reaction heat at the interface between the electrolyte and the cathode particles at time 3000 sec during 1 C discharge process.

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