

Perspectives on Factors Controlling Thermal Runaway of Li-ion batteries

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Since their introduction in 1991, lithium-ion batteries have become the dominant rechargeable battery technology for portable products and are beginning to make inroads in transportation and stationary storage applications. Despite the obvious success of Li-ion technology, safety concerns remain. Under suitable triggers, Li-ion cells can undergo venting, vent-with-flame, ejection of cell parts, fire and explosion as the consequence of a process of uncontrolled heat release, termed “thermal runaway”. Safety failures of lithium-ion cells can result from a variety of triggers. Overcharging, overheating, crushing, mechanical impact and external short circuit all represent forms of external triggers (often termed “abuse” conditions) that can lead to safety incidents. Safety concerns have been heightened by highly publicized safety incidents (e.g., the Dreamliner) and ensuing widespread recalls of lithium-ion batteries used in laptop computers and cell phones. The latter failures, which occurred during otherwise normal operation of the cells, are frequently due to development of internal short circuits. At TIAX, we have extensively studied the mechanism of internal short formation through experiments using coin cell as well as 18650 testing. We have found that foreign metal particles present in/on the cathode electrode can dissolve during normal charge/discharge operation and subsequently plate out on the anode. With continued deposition, metal dendrites can grow through the separator and short the cell when the dendrite makes contact with the cathode surface. Based on the insights from this work, we recently announced the development of a sensor technology for detecting incipient internal shorts.

Regardless of the trigger, an improved understanding of the factors governing thermal runaway can result in the development of technologies to enable safer Li-ion batteries. At TIAX, we have been combining experiments with modeling to improve our understanding of the factors that influence thermal runaway. We have custom-designed and fabricated 18650 cells with a wide range of anode and cathode materials. One such experiment is shown in Figure 1 using an 18650 cell with NCA cathode and graphite anode that we fabricated in our prototyping facility.

We have validated an FEA model for thermal runaway of L-ion cells using data such as that given in Figure 1. Critical inputs to the model are the kinetics of thermal decomposition reactions at the anode and cathode. These were first measured in careful differential scanning calorimetry (DSC) experiments. These kinetic data were then fit with representative numerical models, which were then used in the FEA model. As an example, the model fit for the charged graphite anode in contact with the electrolyte is shown in Figure 2. We are exercising this validated model to ask a series of what-if questions with regard to the influence of cell design factors and environmental factors on the propensity for thermal runaway following a trigger.

In this presentation, we will review the current understanding of the safety of Li-ion batteries. We will discuss the various triggers and how they initiate thermal

runaway. We will describe the approach we have used for validating our FEA model, including custom experiments using cells fabricated in our prototyping facility. We will discuss the results of sensitivity analyses with the validated model to outline the relative importance of cell design factors and environmental factors (such as cell size, active material composition, external and internal heat transfer conditions) in determining thermal runaway of Li-ion batteries.

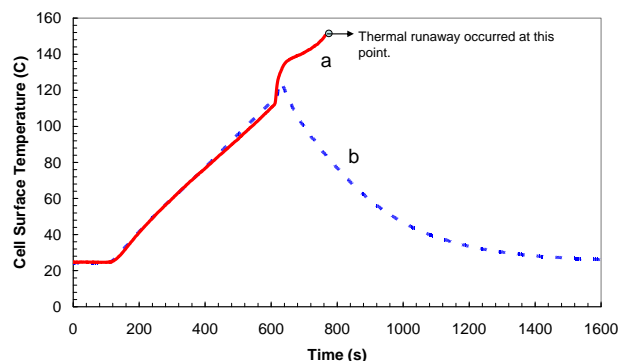


Figure 1: Experimental assessment of the effect of the surface heat transfer coefficient on the propensity for thermal runaway. 18650 cells were fabricated in our prototyping facility with NCA/graphite and modified with miniature heater inserts to achieve localized, controllable internal heating. For the first experiment (curve a), the external heat transfer coefficient and the power dissipated through the heater were set at baseline values, and the cell experienced thermal runaway when its surface temperature exceeded 150°C. (Further temperature data were not recorded because the thermocouple came loose due to the violence of the thermal runaway event.) For the second experiment (curve b), initial heat transfer coefficient and heater power were also set to baseline values. However, when the cell surface temperature reached 120°C, the external heat transfer coefficient was increased by a factor of 4 without any change in the heater power, effectively quenching the progression towards thermal runaway. This type of data was used for validating our FEA thermal runaway model.

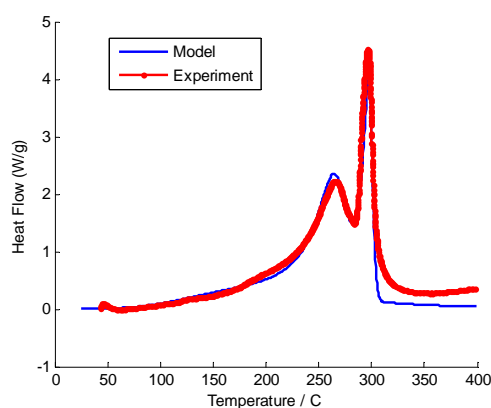


Figure 2: Model fit to the experimentally obtained differential scanning calorimetry (DSC) data for charged graphite anode material in contact with electrolyte. The anode used in this experiment was the same as the anode employed in the cell used for the experiment in Figure 1. The model parameters used for fitting the DSC data were used as inputs to the FEA model for simulating the thermal runaway shown in Figure 1.