Materials

Optimized Li-Ion Electrolytes Containing Fluorinated Ester Co-Solvents

Resulting rechargeable batteries could be used in consumer electronics, electric cars, and scientific instrumentation in extreme environments.

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A number of experimental lithium-ion cells, consisting of MCMB (meso-carbon microbeads) carbon anodes and $LiNi_{0.8}Co_{0.2}O_2$ cathodes, have been fabricated with increased safety and expanded capability. These cells serve to verify and demonstrate the reversibility, low-temperature performance, and electrochemical aspects of each electrode as determined from a number of electrochemical characterization techniques. A number of Li-ion electrolytes possessing fluorinated ester co-solvents, namely trifluoroethyl butyrate (TFEB) and trifluoroethyl propionate (TFEP), were demonstrated to deliver good performance over a wide temperature range in experimental lithium-ion cells.

The general approach taken in the development of these electrolyte formulations is to optimize the type and composition of the co-solvents in ternary and quaternary solutions, focusing upon adequate stability [i.e., EC (ethylene carbonate) content needed for anode passivation, and EMC (ethyl methyl carbonate) content needed for lowering the viscosity and widening the temperature range, while still providing good stability], enhancing the inherent safety characteristics (incorporation of fluorinated esters), and widening the temperature range of operation (the use of both fluorinated and non-fluorinated esters). Furthermore, the use of electrolyte additives, such as VC (vinylene carbonate) [solid electrolyte interface (SEI) promoter] and DMAc (thermal stabilizing additive), provide enhanced high-temperature life characteristics.

Multi-component electrolyte formulations enhance performance over a temperature range of –60 to +60 ºC. With the need for more safety with the use of these batteries, flammability was a consideration. One of the solvents investigated, TFEB, had the best performance with improved low-temperature capability and high-temperature resilience. This work optimized the use of TFEB as a co-solvent by developing the multi-component electrolytes, which also contain non-halogenated esters, film forming additives, thermal stabilizing additives, and flame retardant additives.

Further optimization of these electrolyte formulations is anticipated to yield improved performance. It is also anticipated that much improved performance will be demonstrated once these electrolyte solutions are incorporated into hermetically sealed, large capacity prototype cells, especially if effort is devoted to ensure that all electrolyte components are highly pure.

Probabilistic Multi-Factor Interaction Model for Complex Material Behavior

Complex material behavior is represented by a single equation of product form.

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Complex material behavior is represented by a single equation of product form to account for interaction among the various factors. The factors are selected by the physics of the problem and the environment that the model is to represent. For example, different factors will be required for each to represent temperature, moisture, erosion, corrosion, etc. It is important that the equation represent the physics of the behavior in its entirety accurately.

The Multi-Factor Interaction Model (MFIM) is used to evaluate the divot weight (foam weight ejected) from the external launch tanks. The multi-factor has sufficient degrees of freedom to evaluate a large number of factors that may contribute to the divot ejection. It also accommodates all interactions by its product

form. Each factor has an exponent that satisfies only two points — the initial and final points. The exponent describes a monotonic path from the initial condition to the final. The exponent values are selected so that the described path makes sense in the absence of experimental data. In the present investigation, the data used were obtained by testing simulated specimens in launching conditions. Re-

sults show that the MFIM is an effective method of describing the divot weight ejected under the conditions investigated.

The problem lies in how to represent the divot weight with a single equation. A unique solution to this problem is a multi-factor equation of product form. Each factor is of the following form $(1 - x_i/x_f)^{q_i}$, where x_i is the initial value, usually at ambient conditions, x_f the final value, and e_i the exponent that makes the curve represented unimodal that meets the initial and final values. The exponents are either evaluated by test data or by technical judgment. A minor disadvantage may be the selection of exponents in the absence of any empirical data. This form has been used successfully in describing the foam ejected in simulated space environmental conditions. Seven factors were required to represent the ejected foam. The exponents were evaluated by least squares method from experimental data.

The equation is used and it can represent multiple factors in other problems as well; for example, evaluation of fatigue life, creep life, fracture toughness, and structural fracture, as well as optimization functions. The software is rather simplistic. Required inputs are initial value, final value, and an exponent for each factor. The number of factors is open-ended. The value is updated as each factor is evaluated. If a factor goes to zero, the previous value is used in the evaluation.