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 (mesocarbon 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 °C. 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.

This work was done by G. K. Surya Prakash of the University of Southern California and Marshall Smart, Kiah Smith, and Ratnakumar Bugga of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).

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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-