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Lithium Ion Batteries with Improved Performance and Safety

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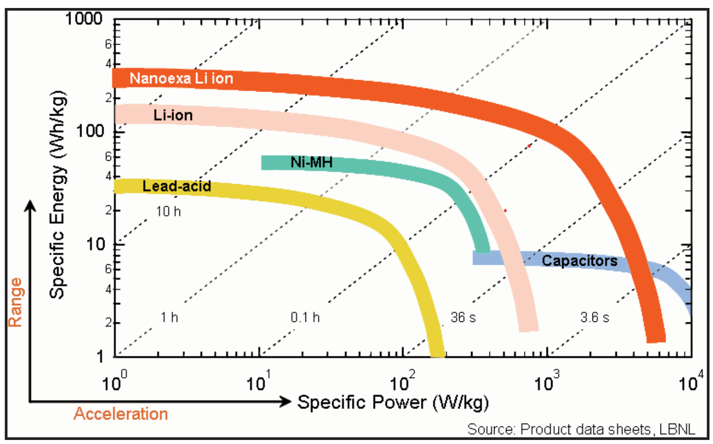
While battery technology advancement has generally lagged behind other technology sectors such as semiconductors, recent advances in lithium batteries, particularly at the material level, suggest that batteries will be vastly improved in the near future. This signifies a tremendous shift in the battery industry and it offers promise for so many applications that desire better batteries, particularly vehicles. Previously, other types of batteries such as Nickel Metal Hydride, Nickel Cadmium, and Lead Acid batteries were used by many applications because lithium based batteries were either too expensive, unsafe or unreliable. Now, with new battery materials, new generations of lithium batteries are being developed that are less expensive, safer and provide better performance than previous generations of lithium batteries. One company on the forefront of developing these new lithium batteries is Nanoexa. The company, located in Silicon Valley, has partnered with Argonne National Laboratory to manufacture high power and high energy lithium ion batteries for power tools, hybrid electric vehicles and pure electric vehicles.

Battery Basics

Despite being first developed in the early 1900's, lithium batteries did not reach the commercial market until the 1990's, where they began their dominance in the mobile market primarily because of their ability to have very high energy density. But even though lithium batteries are the most relevant batteries to our daily lives, namely mobile phones and laptops, the battery market in general is still dominated by older chemistries. Lead acid batteries are appealing to a lot of industrial applications because they are reliable, inexpensive, and safe. On the down side, they have low cycle life and low energy density (30 to 45 Wh/kg), making them unattractive for all power hungry applications. Nickel Cadmium (NiCd) batteries have been used in consumer electronics and power tools because of their tolerance for abuse and their high cylclibility, but they suffer from low energy density in addition to the negative environmental impact surrounding cadmium. Nickel Metal Hydride (NiMH) batteries have higher energy density (60 to 110 Wh/kg) than NiCd and Lead Acid batteries as well as higher power densities. While NiMH batteries are experiencing resurgence in demand as a result of growing hybrid electric vehicle (HEV) market, they have high self-discharge rates and they are inferior to lithium ion batteries in term of power and energy density.

Lithium batteries have been popular in applications that require high energy density, such as portable devices, but are historically more expensive than all other popular battery systems. Lithium batteries are also still considered more dangerous and less robust than other battery systems. The negative features of lithium batteries, including cost, can be more simply attributed to the fact that it is a relatively new technology, whereas other battery chemistries are much more mature. The truth is that lithium batteries have witnessed a doubling in volumetric energy density over the past ten years and the price per watt hour (Wh) is 6 times less today than it was 10 years ago. Lithium batteries have advanced with relatively little change in material composition and structure. Nanoexa is useing computational modeling to invent new battery materials.



New Materials for Better Lithium Batteries

Carbon, typically in the form of graphite and LiCoO2 (both of which have layered structures) have remained the electrode material of choice in almost all commercial lithium batteries in use today. Layered LiCoO2 is not a stable structure especially when it is delithiated and can decompose, which liberates oxygen. The exothermic reactions can escalate in high temperatures, causing a positive-feedback effect called "thermal runaway." Not surprisingly, most of the batteries that have been recalled in recent times have contained a LiCoO2 positive electrode, in addition to a carbon negative electrode and an organic lithium ion conducting electrolyte

In order for lithium batteries to continue performance improvements, it is absolutely necessary to utilize different materials for the cathode, anode and electrolyte. Cell design can only produce incremental improvements whereas material composition and morphology can provide huge leaps in performance. For lithium batteries there are a few new cathode and anode materials that have demonstrated potential. One cathode material, originally developed by Argonne National Laboratory, is now being commercialized in batteries by Nanoexa. These batteries are based on a new composition and new crystal structure developed at Argonne National Laboratory. The positive electrode has a layered-layered composite crystal structures in which a Li2MnO3 (layered) component is structurally integrated with layered LiMO2. The electrodes can be represented in two-component notation as xLi2MnO3 o (1-x)LiMO2 where M is from group Ni, Mn, Co. Li2MnO3 (layered) component is structurally integrated with layered LiMO2. What makes Nanoexa's approach unique is not the materials used (nickel, cobalt and manganese), as others have experimented with this composition, rather the crystal structure in which these materials are arranged, which has been coined 'layered-layered' by its inventors at Argonne National Laboratory.

In this composite structure, Li2MnO3 is electrochemically inactive but stabilizes the electrochemically active LiMO2. It also reduces the oxygen activity at the surface of the charged electrode particles further enhancing the safety of the system. These electrodes are very stable and show no oxygen release under typical operating conditions. The safety characteristics of Nanoexa's batteries have been verified using accelerated rate calorimetric test.

Computational Modeling For Lithium Batteries

Nanoexa is the first company to utilize computational modeling to invent new materials for lithium batteries. In addition to its unique cathode material structure that offers improved performance and safety, Nanoexa uses computational modeling to further enhance its material design and optimize the overall battery system through a deep understanding of the electrochemistry of materials at the quantum level. Computational modeling techniques will be able to rapidly screen new cathode, anode and electrolyte materials and select only those with promise.

Within the realm of computational modeling, Nanoexa has initially utilized what is known as first-principles computation or ab initio calculations. First principles computation, whereby the properties of materials are predicted starting from the principles of quantum mechanics and density functional theory, has become integral part of traditional materials research. Successful first-principles methods can bring obvious advantages to materials research because no experimental input is needed, and the behavior of a material can be predicted before it is synthesized, making it possible to quickly focus on only the promising designs.

Nanoexa has simulated several cathodes materials currently being used in Li-ion battery. We have calculated a number of different material properties, such as lattice parameters and total energies, which then enable us to provide data that could previously only be found experimentally such as the x-ray diffraction (XRD) pattern. Computer simulation also increases our understanding and helps improve power, capacity, safety, cycling properties and temperature performance of these materials.

Enabling Applications

It is Nanoexa's objectives to create batteries that enable new applications and displace older battery chemistries used in high growth application sectors. Nanoexa's battery technology will meet the battery goals of the US Advanced Battery Consortium (USABC) FreedomCAR performance goals for HEVs. Generally speaking, most lithium batteries can meet some of the requirements, but current commercial batteries usually fall short on power, calendar life, cyclibility or safety. Nanoexa's batteries have successfully addressed each of these categories.

Nanoexa has developed cylindrical cells with high power and high energy density for power tool applications. The first product is an 1,700 mAh 18650 cell capable of discharging at high rates suitable for power tools. The company's first prototypes have demonstrated a cycle life of over 300 while retaining 80 percent of their original capacity when discharged continuously at 10C rate. The prototype cells performed well under low temperature testing at -20°C, as they retained more than 60 percent of the original capacity when discharged at high rates. Currently, the design for 26,650 cells is under way capable of having capacity up to 3,100 mAh when discharged at 10 C rate.

But power and energy are just a couple pieces of overall battery performance. Unlike mobile devices, where battery life is not a crucial attribute, automobile makers prefer to have a battery life of at least 10 years. To improve calendar life, Nanoexa incorporates an electrolyte additive that prevents cell impedance from growing over time. Normally, the steady growth in cell impedance limits Li-ion battery life to about five years. However, use of the additive is expected to extend battery life to 15 years.

Similarly, the recent laptop recalls due to dangerous or defective batteries has not only increased the fear of lithium batteries, it has also made safety a paramount concern when a new application adopts a new battery. Since lithium batteries use flammable organic solvent with a relatively low flash point, thermal runaway can lead to fire and explosion. Nanoexa has further enhanced the safety of its batteries using proprietary additives that make electrolytes totally non-flammable. This will allow complete safety of batteries even under abusive condition. In an effort to curtail the potential of thermal runaway, Nanoexa has developed Lithium ion batteries with inherently safer electrodes and non-flammable electrolytes, which prevents the battery from catching fire.

While lithium battery technology has advanced somewhat incrementally, battery components are now being optimized to create inexpensive, safe, high performance batteries that can now displace older technologies. Like the activation barrier in a chemical reaction, batteries developed by Nanoexa have reached the tipping point where they can successfully enable automobile applications like HEV for the mass markets.

Contact Nanoexa at www.nanoexa.com.