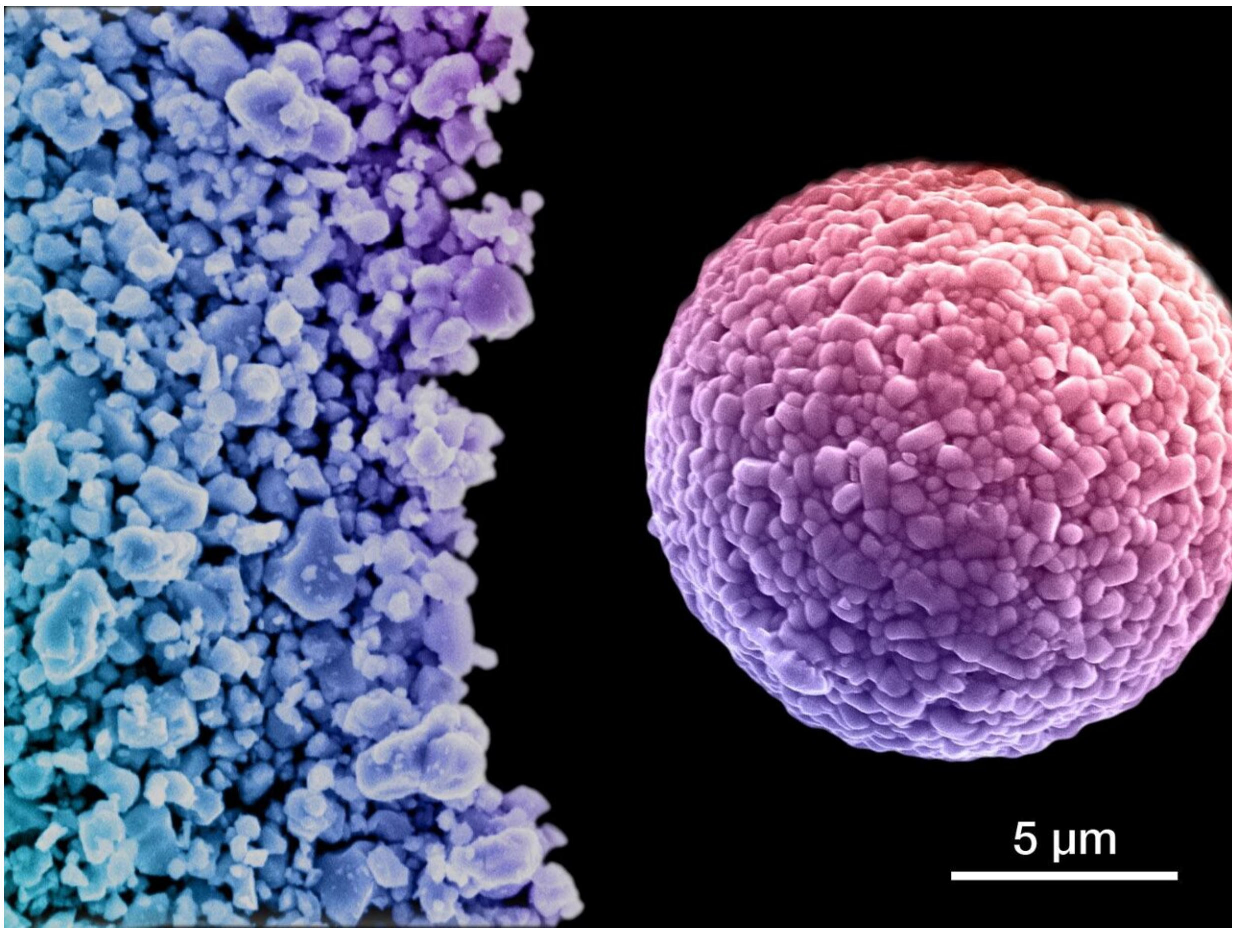
More range for electric vehicle batteries on the horizon

December 13 2023, by Oliver PeckhamOliver Peckham



Single-crystal structures for cathode materials (left) are juxtaposed with an agglomerated polycrystal structure (right).. Credit: Composite image by Nathan Johnson, Pacific Northwest National Laboratory

A seemingly simple shift in lithium-ion battery manufacturing could pay big dividends, improving electric vehicles' (EV) ability to store more energy per charge and to withstand more charging cycles, according to new research led by the Department of Energy's Pacific Northwest National Laboratory.

An EV's mileage depends on the deliverable energy from each of the constituent cells of its battery pack. For lithium-ion cells—which dominate the EV battery market—both the cell-level energy capacity and the cell cost are bottlenecked by the positive electrode, or cathode.

Now that bottleneck might be opening up, thanks to an innovative, cost-effective approach for synthesizing single-crystal, high-energy, nickel-rich cathodes that was recently published in *Energy Storage Materials*.

The nickel-rich battery vision

Cathodes for conventional EV batteries use a cocktail of metal oxides—lithium nickel manganese cobalt oxides ($LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$), abbreviated NMC. When more nickel is incorporated into a cathode, it greatly increases the battery's ability to store energy, and thus, the range of the EV. As a result, nickel-rich NMC (such as NMC811, where the "8" denotes 80% nickel) is of great interest and importance.

However, high-nickel NMC cathodes formed using the standard method are agglomerated into polycrystal structures that are rough and lumpy. This meatball-like texture has its advantages for regular NMC. For NMC811 and beyond, though, the bulbous polycrystal fissures are prone to splitting apart, causing material failure. This renders batteries made using these nickel-rich cathodes susceptible to cracking; they also begin to produce gases and decay faster than cathodes with less nickel.

Challenges of synthesizing single-crystal NMC811

One strategy to fix this problem: convert that lumpy, polycrystal NMC into a smooth, single-crystal form by eliminating the problematic boundaries between the crystals—but this conversion is easier said than done. In laboratories, single crystals are grown in environments such as molten salts or hydrothermal reactions that produce smooth crystal surfaces. However, these environments are not practical for real-world cathode manufacturing, where lower-cost, solid-state methods are preferred.

In these more typical solid-state approaches, an NMC cathode is prepared by mixing a metal hydroxide precursor with lithium salt, directly mixing and heating those hydroxides—and producing the agglomerated (lumpily clustered) polycrystal NMC. Using a multiple-step heating process results in micron-sized crystals—but they are still agglomerated, so the undesirable side effects persist.

The solution

Led by PNNL battery experts, and in collaboration with Albemarle Corporation, the research team solved these issues by introducing a pre-heating step that changes the structure and chemical properties of the transition metal hydroxide. When the pre-heated transition metal hydroxide reacts with lithium salt to form the cathode, it creates a uniform single-crystal NMC structure that looks smooth, even under magnification.

"The one-step heating process of precursors seems straightforward, but there is a lot of interesting atomic-level phase transition involved to make the single crystal segregation possible," said Yujing Bi, first author of the paper. "It is also convenient for industry to adopt."

In their study, the researchers are now scaling up this single-crystal NMC811 to kilogram level by using lithium salt provided by Albemarle. The scaled single crystals were tested in realistic 2Ah lithium-ion pouch cells, using a standard graphite anode to make sure that the battery's performance was mainly dictated by the new cathode.

The first prototype battery equipped with the scaled single crystals was stable, even after 1,000 charge and discharge cycles. When the researchers looked at the microscopic structure of the crystals after 1,000 cycles, they found no defects and a perfectly aligned electronic structure.

"This is an important breakthrough that will allow the highest energy density lithium batteries to be used without degradation," commented Stan Whittingham, a Nobel Laureate and distinguished professor of chemistry at Binghamton University. "In addition, this breakthrough on long-lived batteries will be critical to their use in vehicles that can be tethered to the grid to make it more resilient and to support clean renewable energy sources."

The synthesis method for the single-crystal, nickel-rich cathode is both innovative and cost-efficient. It is also easy to scale up, as it is a drop-in approach that allows cathode manufacturers to use existing production facilities to conveniently produce single-crystal NMC811—and even cathodes with more than 80% nickel.

"This is a fundamentally new direction for large scale production of single crystal cathode materials," said Jie Xiao, the principal investigator of the project and a Battelle Fellow at PNNL. "This work is only part of the cathode technology we are developing at PNNL. In collaboration with Albemarle, we are addressing the scientific challenges in synthesis and scaleup of single crystals and reducing the manufacturing cost starting from raw materials."

Rapid deployment of EV battery technology

In the research phase, set to begin in early 2024, PNNL, teaming up with industry and university partners, will work to realize commercial-scale synthesis and testing with an eye toward production.

To accomplish this so quickly, they will use conventional manufacturing equipment and techniques that have been industrially adapted to include PNNL's scale-up approach (as well as a few other innovations that further reduce costs and waste generation).

"During single-crystal synthesis at the kilograms level, we have identified a brand new world full of science and engineering challenges and opportunities," said Xiao. "We are excited to apply this new knowledge to accelerate the commercial-scale manufacturing process."

"We are not competing with industry," said Xiao. "In fact, we are partnering with industry leaders like Albemarle to proactively address the scientific challenges so that industry can scale up the whole process based on the lessons and knowledge that we learned along the way."

More information: Yujing Bi et al, Simultaneous Single Crystal Growth and Segregation of Ni-Rich Cathode Enabled by Nanoscale Phase Separation for Advanced Lithium-Ion Batteries, *Energy Storage Materials* (2023). DOI: 10.1016/j.ensm.2023.102947

Provided by Pacific Northwest National Laboratory