Single-crystal synthesis technology enhances durability of lithium secondary batteries

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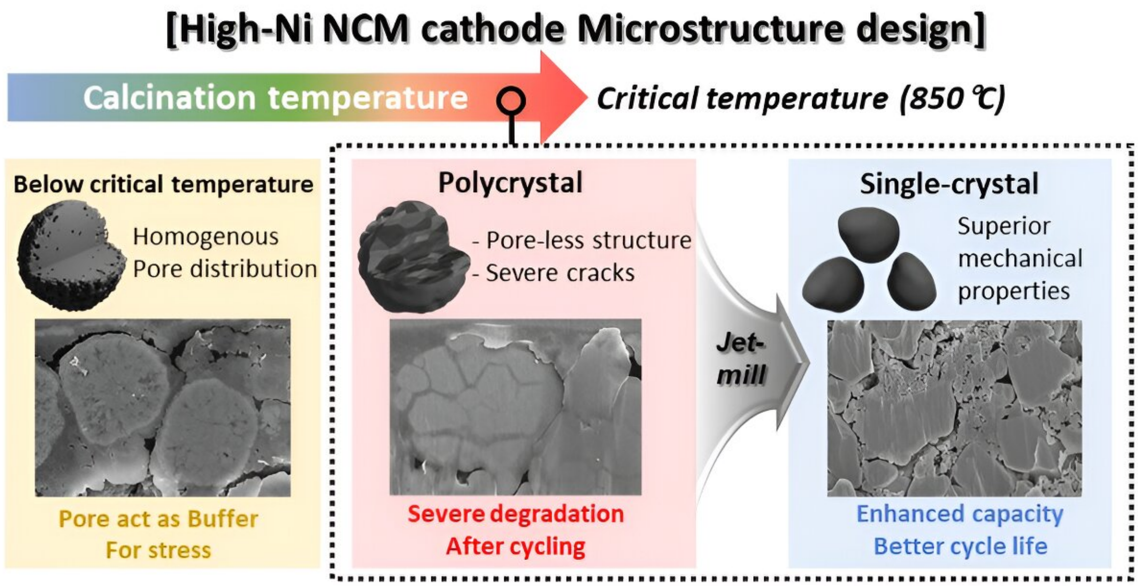

Schematic of the microstructure evolution of high-nickel cathode materials with synthesis temperature and a strategy for synthesizing single crystals at a critical temperaturete. Credit: POSTECH

A research team has recently demonstrated a single-crystal synthesis technology that significantly extends the lifespan of cathode materials for electric vehicles. This research was published in the online edition of *ACS Materials & Interfaces*, an international journal in the materials science field.

Lithium (Li) secondary batteries, commonly used in electric vehicles, store energy by converting electrical energy to chemical energy and generating electricity to release chemical energy to electrical energy through the movement of Li- ions between a cathode and an anode. These secondary batteries mainly use nickel (Ni) cathode materials due to their high lithium-ion storage capacity. Traditional nickel-based materials have a polycrystalline morphology composed of many tiny crystals which can undergo structural degradation during charging and discharging, significantly reducing their lifespan.

One approach to addressing this issue is to produce the cathode material in a "single-crystal" form. Creating nickel-based cathode materials as single large particles, or "single crystals," can enhance their structural and chemical stability and durability. It is known that single-crystal materials are synthesized at high temperatures and become rigid. However, the exact process of hardening during synthesis and the specific conditions under which this occurs remain unclear.

To improve the durability of nickel cathode materials for electric vehicles, the researchers focused on identifying a specific temperature, referred to as the "critical temperature," at which high-quality single-crystal materials are synthesized. They investigated various synthesis temperatures to determine the optimal conditions for forming single crystals in synthesis of a nickel-based cathode material (N884). The team systematically observed the impact of temperature on the material's capacity and long-term performance.

The researchers discovered that conventional polycrystalline materials synthesized below a certain critical temperature are prone to degradation with prolonged use in secondary batteries. However, when synthesized above this critical temperature, high-quality single crystals can be easily produced, leading to materials with superior longevity. This is due to a process called "densification" which occurs above a certain critical temperature.

During this process, the internal grain size of the material increases and the empty spaces within the material are densely filled. Densified single crystals are extremely hard and resistant to degradation over extended periods, significantly enhancing their durability. Based on these findings, the team confirmed that synthesizing single crystals above the critical temperature is a more advantageous material design strategy. They also proposed an effective method for synthesizing high-quality single crystal materials.

The team was led by Professor Kyu-Young Park from the Graduate Institute of Ferrous & Eco Materials Technology and the Department of Materials Science and Engineering and Kyoung Eun Lee, a Ph.D. candidate, and alumna Yura Kim from the Graduate Institute of Ferrous & Eco Materials Technology at Pohang University of Science and Technology (POSTECH), in collaboration with the POSCO Holdings N.EX.T Hub.

Professor Park of POSTECH stated, "We have introduced a new synthesis strategy to enhance the durability of nickel-based cathode materials. We will continue our research to make secondary batteries for electric vehicles cheaper, faster, and longer-lasting."

More information: Kyoung Eun Lee et al, Comparison Study of a Thermal-Driven Microstructure in a High-Ni Cathode for Lithium-Ion Batteries: Critical Calcination Temperature for Polycrystalline and Single-Crystalline Design, *ACS Applied Materials & Interfaces* (2024). DOI: 10.1021/acsami.4c00514

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