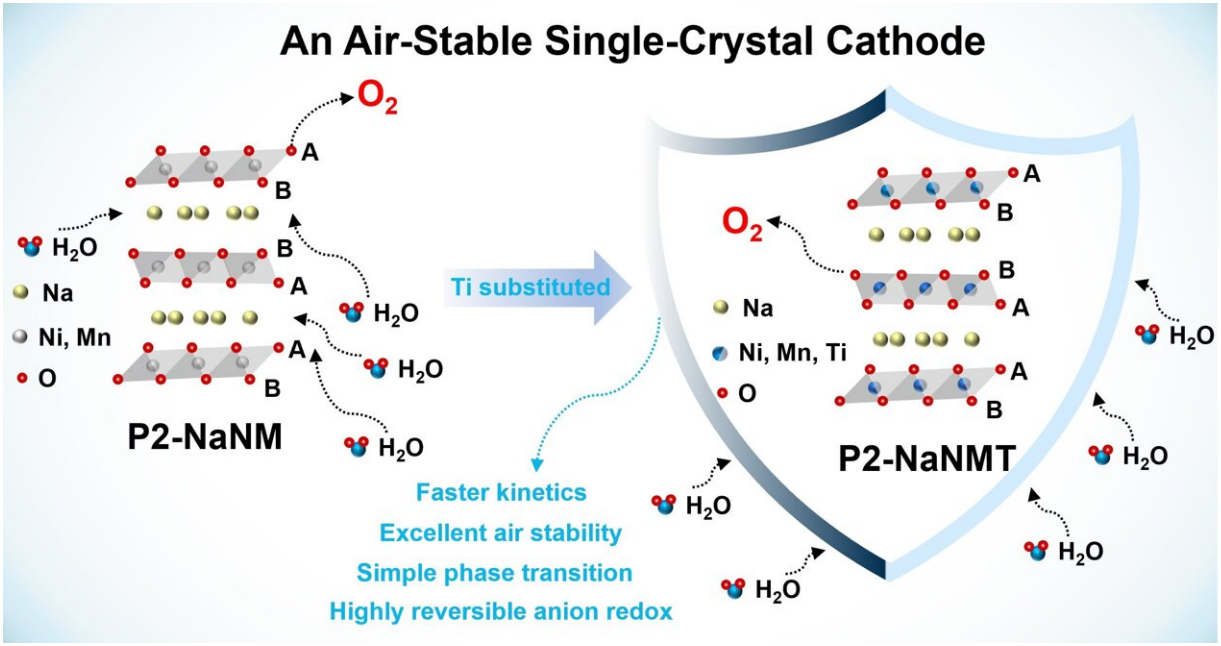
An air-stable single-crystal layered oxide cathode based on multifunctional structural modulation

March 20 2024



Enhancement mechanism of multifunctional structural modulation strategy based on Ti substitution. Credit: Science China Press

Sodium-ion batteries (SIBs) are considered a promising energy storage system due to their superior safety properties, low price, and plentiful sodium supplies, while the development of electrode materials plays a critical function in the performance of SIBs.

P2-$Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ is a typical layered oxide cathode material for SIBs, characterized by its unique structural features that provide rapid ion transport pathways and lower diffusion barriers for Na^+ ions. Consequently, it has garnered significant attention from numerous researchers.

However, this material also faces challenges such as complex multiphase transition and irreversible anion redox processes, which limit its electrochemical performance. Therefore, there is an urgent need to develop effective strategies for modifying this material to enhance its practicality.

Now, in a recent study published in *Science China Chemistry*, led by Professor Yao Xiao from the College of Chemistry and Materials Engineering at Wenzhou University, a team of researchers has proposed a strategy of Ti-substituted-boosting the single crystalline growth and designed a hydrostable ~10 μm single-crystal P2-$Na_{2/3}Ni_{1/3}Mn_{1/3}Ti_{1/3}O_2$ cathode material as the prototype.

"According to Vegard's law, the lattice parameter is changed by the constituents with similar absolute Vegard's slope of the system. Otherwise, the concentrated dopants can migrate to the surfaces and create an eutectic film that has a lower melting point than the two pure components, which is beneficial to the interface atomic diffusion and crystal growth. Therefore, it is reasonable to suspect that Ti^{4+} with larger Vegard's slopes could promote the crystal growth of cathodes," Xiao says.

The study focused on the formation process, electrochemical behavior, structural evolution, and air stability of P2-$Na_{2/3}Ni_{1/3}Mn_{1/3}Ti_{1/3}O_2$ through advanced characterization techniques, and explored the relationship between its structure, function, and properties.

The results showed that the substitution of Ti is beneficial to generating large-size grains, suppressing multiple phase transitions, and inhibiting irreversible anion redox through structural regulation. The obtained material not only shows a high energy density and delivers good cycle performance but also greatly improves Na^+ transport kinetics and air stability.

Overall, this study may provide insights into multifunctional structural modulation for the development of high-performance sodium-based layered cathode materials for practical applications.

More information: Yi-Feng Liu et al, An air-stable single-crystal layered oxide cathode based on multifunctional structural modulation for high-energy-density sodium-ion batteries, *Science China Chemistry* (2024). DOI: 10.1007/s11426-023-1891-4

Provided by Science China Press