Application Note BATT1027

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BATT1027: Evaluation of nanoscale structural changes in primary particles of NCM by electron diffraction

Introduction

While NCM cathode materials contribute to high capacity, repeated cycles can cause strain and lattice disorder to accumulate inside the particles, leading to rapid performance degradation. Although it was previously difficult to directly observe the causes of such changes at the nanoscale, fully evaluating the three-dimensional extent of each Bragg reflection in electron-beam diffraction now makes it possible to treat each sub-micron-sized NMC particle as a single crystal and obtain highly accurate structural information. This enables the acquisition of high-precision structural information. Furthermore, it is possible to quantitatively understand where and how the strains, defects, and lattice distortions that occur in NCM cathode particles after charging and discharging change on a nanoscale.

Crystal phase analysis

- **Analysis:** Cathode material
- **Use:** Optimizing electrochemical performance
- **Analyzed materials:** $LiNi_xCo_yMn_zO_2$, NCM

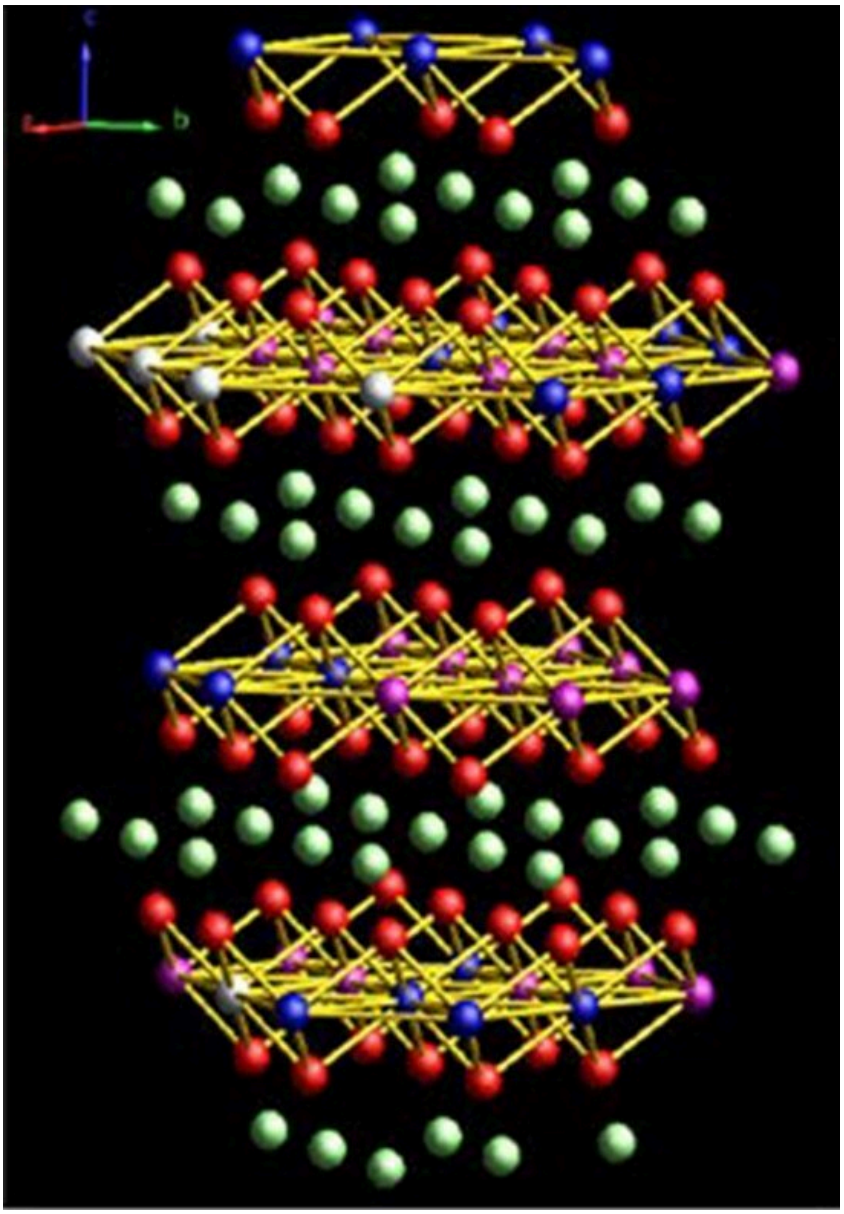
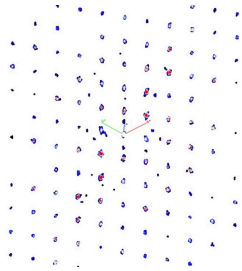
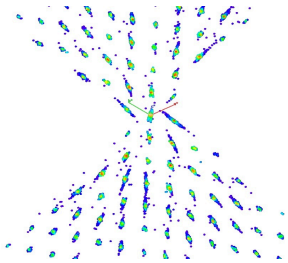


Figure 1: Crystal structure of NCM



Initial particles



Post-cycle particles

Figure 2: Diffraction peaks of reciprocal lattice

Conclusion

Three-dimensional structural analysis of individual NCM primary particles by electron diffraction revealed clear structural changes after charge-discharge cycles. Initially, the diffraction peaks in reciprocal lattice space were mainly circular, but after charge-discharge cycling, the peaks were elongated, suggesting increased lattice distortion and structural disorder.

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User-inspired data collection and data processing software for small molecule and protein crystallography.

XtaLAB Synergy-ED

A new and fully integrated electron diffractometer for meas uring submicron crystals, utilizing a seamless workflow fro m data collection to structure determination of crystal struc tures.