Battery materials research and quality control solutions

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ABSTRACT

$LiFePO_4$, normally referred to as LFP, is a major cathode material used by lithium-ion battery industry. LFP has its advantage in superior safety and lower material cost compared to other popular chemistries like NMC ($LiNi_xMn_yCo_{1-x-y}O_2$). Although LFP has lower energy density compared to NMC, this gap is diminishing fast with new battery manufacturing and assembling techniques, like Cell to Pack (CTP) and blade battery designs.

The critical parameters, which influence the battery performance, are primary particle size and crystalline phases of the electrode materials. X-ray diffraction (XRD) is a non-destructive technique routinely used for the identification of crystalline phases. The Rietveld method[1] is an established method used for the analysis of powder XRD data, allows to refine the crystallographic structures of the synthesized materials, quantify the amount of each phase in the bulk and characterise the average crystallite size and microstrain. The extracted crystallographic information such as interlayer spacing can be used to calculate the degree of graphitization or the orientation index in graphite battery anode materials.

Although average crystallite size can be extracted from powder XRD data, it is not always equal to the primary particle size, crucial for cathode performance. The combination of X-ray diffraction with laser diffraction and dynamic light scattering techniques comprises a comprehensive approach to the characterisation of size parameters over a large size range.

In this study, we will investigate the Li-ion battery, LMFP (LiMnxFe1-x(PO4)) cathode materials with the Mn content varying from 0 to 0.8, and some synthetic graphite (anode) samples using powder XRD. The correlation of the average crystallite size, determined by XRD, with the particle size measurements by laser diffraction and dynamic light scattering is also discussed.

REFERENCES:

[1] H. M. Rietveld. *J. Appl. Cryst*. **1969**, *2*, 65