Application Note BATT1012

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BATT1012 - Inference of Valence and Li Ion Diffusion Path Using the BVS Method

Introduction

The valence of general cathode materials affects battery performance. For that reason, they are analyzed using XAFS and ESCA. Using the BVS method, it is possible to infer valence based on interatomic distances with XRD. Additionally, by applying the BVS method it is possible to infer the diffusion path by determining the interatomic distance at which it is easy for Li ions to become monovalent.

Crystal phase analysis

- **Analysis:** Cathode material
- **Analysis method:** Rietveld analysis, BVS method
- **Use:** Optimizing electrochemical performance
- **Analyzed materials:** $LiFePO_4$, LFP

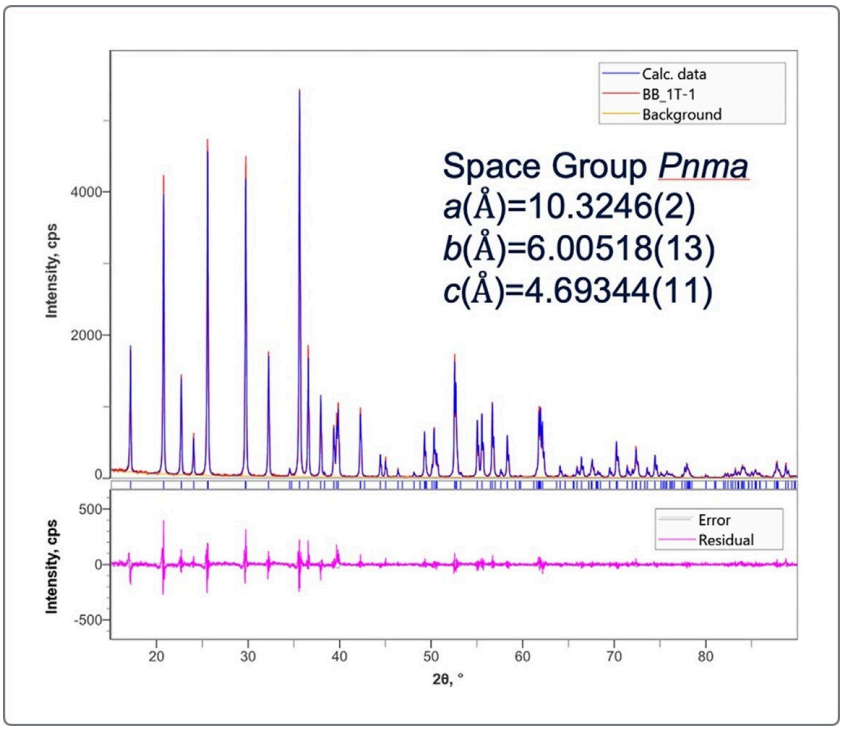

Figure 1: Rietveld analysis results for LFP and lattice constants obtained (R_{wp}:11.13%, S:1.33)

Atoms	*x*	*y*	*z*	Valence According to BVS Method
Li1	0	0	0	0.98
Fe1	0.28231(9)	0.25	0.9744(3)	1.91

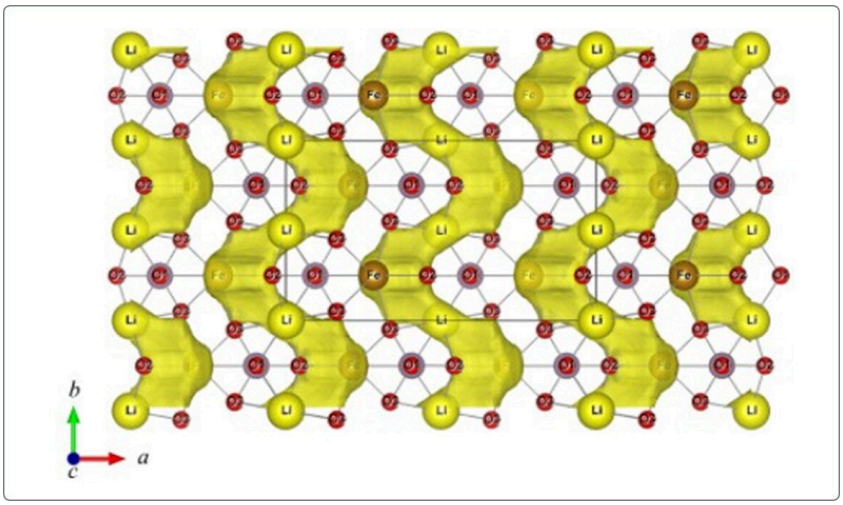

Figure 2: Li and Fe coordinates obtained using Rietveld analysis and valence obtained using the BVS method (top) and Li ion diffusion path inferred using the
BVS method (bottom)
Rendered using VESTA, K. Momma and F. Izumi, "VESTA 3 for three- dimensional visualization of crystal, volumetric and morphology data,"
J. Appl. Crystallogr., 44, 1272-1276 (2011).

Conclusion

Rietveld analysis makes it possible to perform structural analysis. Additionally, using the BVS method, valence and the Li ion diffusion path can be inferred.

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