Phase Analysis of (Li)$FePO_4$ by Selected Area Electron Diffraction in Transmission Electron Microscopy

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Introduction

Lithium iron phosphate ($LiFePO_4$) is a well-studied compound with a lot of promise as cathode material in rechargeable batteries. Due to low cost, low toxicity, safety and the abundance of iron $LiFePO_4$ is considered a very attractive energy storage option for the automotive industry.

To better understand the lithium deintercalation process we performed Selected Area Electron Diffraction (SAED) experiments on chemically and electrochemically (de)lithiated $LiFePO_4$. Single particle diffraction imaging enables us to successfully determine individual phases and delithiation estimate.

Diffraction Results

- Li_xFePO_4 does not change in crystal structure with increasing delithiation grade [1]
- Differences in lattice constants are large enough for electron diffraction!
- SAED patterns are used to map prominent lattice plane distances for small crystallites
- Reference model quality determines precision of the delithiation estimate.

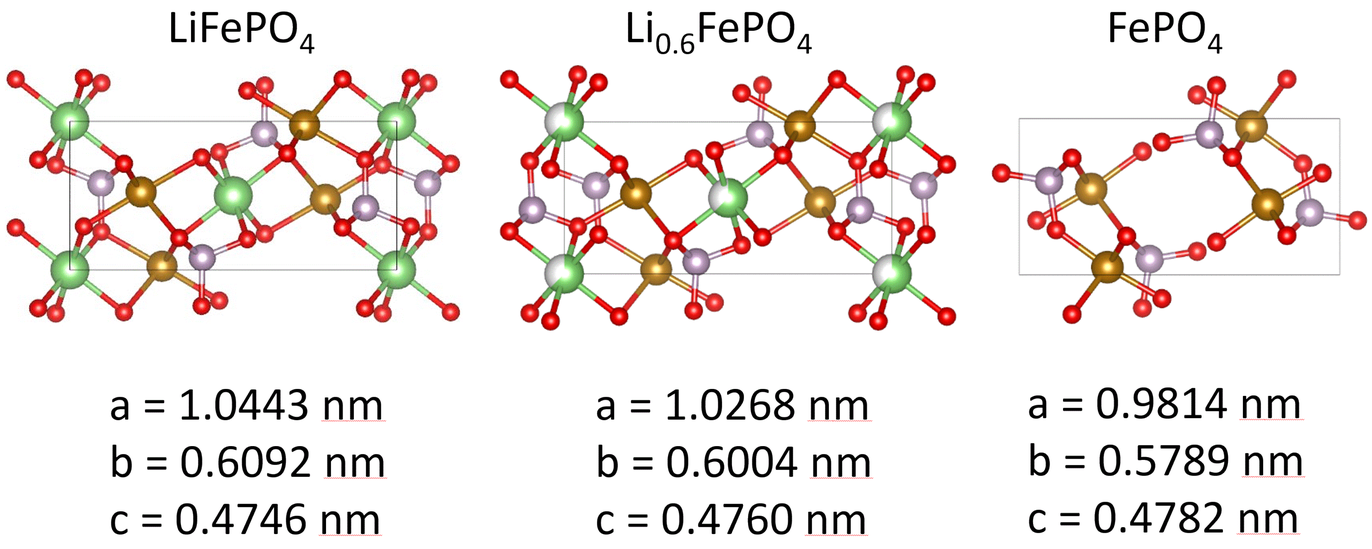

Figure 1: $LiFePO_4$ [2], $Li_{0.6}FePO_4$ and $FePO_4$ reference models [3]. The only difference in the materials is their Li content and lattice constants.

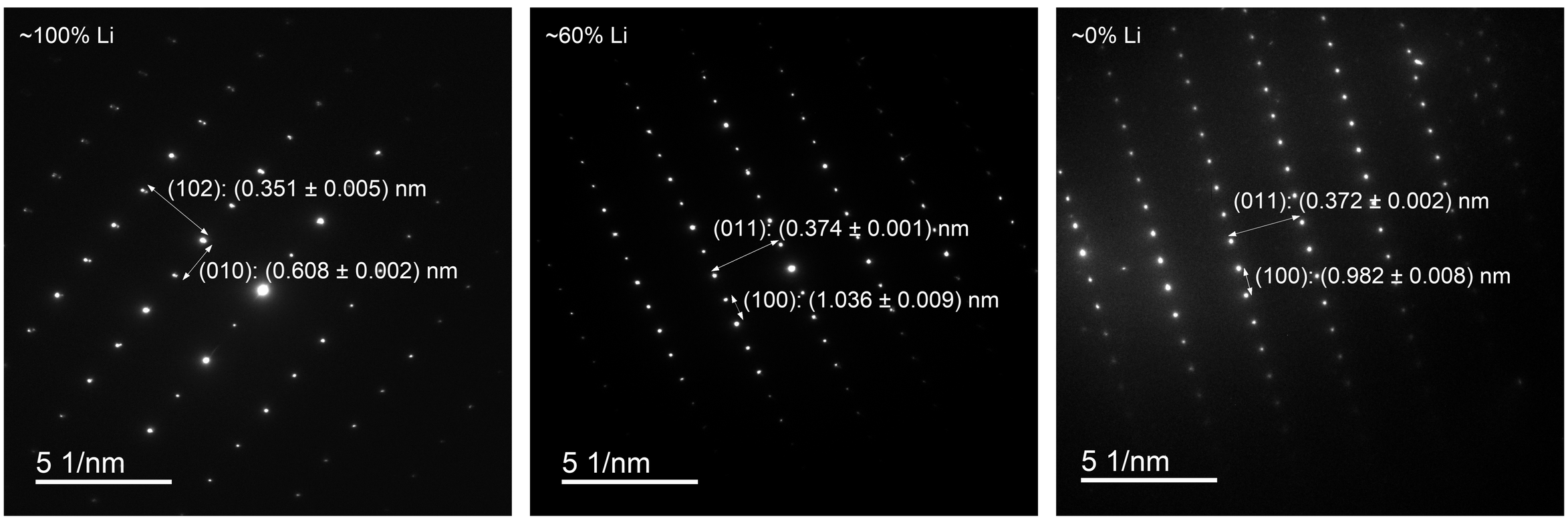

Figure 2: Diffraction Patterns for three crystallites showing $LiFePO_4$, $Li_{0.6}FePO_4$ and $FePO_4$ each.

Conclusion

Selected Area Electron Diffraction is a useful and viable method for phase identification of Li_xFePO_4. Even partial delithiation can be estimated if reference models with the right delithiation grade are available..

References/ Literature

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