

The Delayed Structural Transformation for the LiFePO_4/C during Charging and Discharging at a Lower Rate

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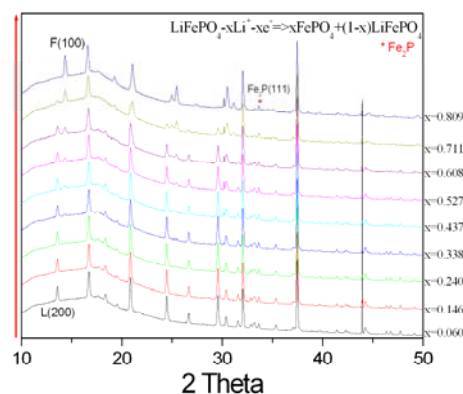
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Figure 1 describes the in-situ synchrotron X-ray diffraction patterns of the LiFePO_4/C synthesized at 800°C during charge and discharge at 0.25C. The reflection peaks, associated with the Fe_2P impurities as the inactive material, were exhibited at 33.6° . The LiFePO_4/C synthesized at 800°C had lower discharging capacity of 135 mAh/g than that synthesized at 750°C at the rate of 0.25C. The lower discharging capacity was affected by a large amount of the Fe_2P impurities. The negative effect of Fe_2P is not yet well known, nevertheless, Song et al. inferred that the formed Fe_2P above the critical concentration disrupted the the one-dimensional Li^+ pathways followed by hindraning Li^+ transport [1]. However, the LiFePO_4/C synthesized at 800°C presented a normal structural transformation process, which was due to the existence of Fe_2P impurities. The impure Fe_2P phase with metallic conductivity of 1.5 S cm^{-1} significantly improved the electronic conductivity of the LiFePO_4 from 10^{-9} to $10^{-3} \text{ S cm}^{-1}$ [2]. The Fe_2P particles might play an important role in affecting the nucleation sites. According to the above-mentioned arguments, the produced Fe_2P phase would disturb the structure of the LiFePO_4 . It was reported that the transportation of Li ions took place near the phase boundary through supplying the activation energy for nucleation [3]. Therefore, the disordered structure, resulted from the Fe_2P phase, possessed more regions with higher energy to stimulate the intercalation and deintercalation of Li ions. Furthermore, the enhanced electronic conductivity of Fe_2P also improved the electron flow to speed the phase transformation.

References

- [1] M.-S. Song, D.-Y. Kim, Y.-M. Kang, Y.-I. Kim, J.-Y. Lee, and H.-S. Kwon, *J. Power Sources* **180**, 546 (2008).
- [2] Y. Xu, Y. Lu, L. Yan, Z. Yang, and R. Yang, *J. Power Sources* **160**, 570 (2006).
- [3] C. Delmas, M. Maccario, L. Croguennec, F. Le Cras, and F. Weill, *Nature mater.* **7**, (2008).

(a)



(b)

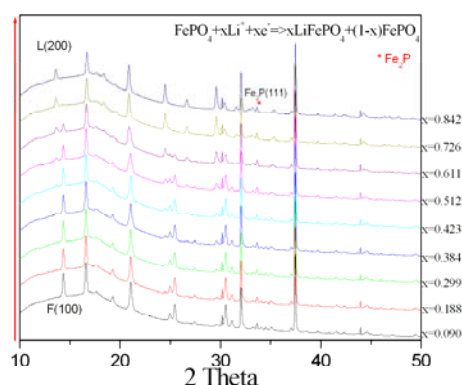


Fig. 1: In-situ X-ray diffraction patterns of LiFePO_4/C synthesized at 800°C (a) charge and (b) discharge at 0.25C ($\lambda=1.334 \text{ \AA}$). The subscripts L and F represent reflections of LiFePO_4 and FePO_4 structures.