

# How Modern Batteries Work: The Effect of Particle Size on Battery Performance

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## Abstract

The purpose of this experiment is to observe how the change in battery structure, specifically cathode material, may amplify or reduce the performance of a coin battery. In this experiment, three different samples of coin batteries were constructed and assembled. In each sample, a different cathode material was used ( $\text{LiFePO}_4$ ,  $\text{FePO}_4 \cdot x\text{H}_2\text{O}$ , and  $\text{FePO}_4 \cdot x\text{H}_8\text{O}$ ). Then, the APS beamline was used to test our samples and observe their different x-ray diffraction patterns or "fingerprints." We used a commercial battery as our control.

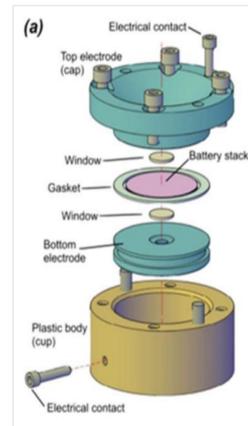
## Background Research

The diffraction pattern shows the difference between the materials because of their different compositions. This allows the different data to be compared to each other. Specifically, the definite structure of the iron phosphate battery which was depicted through its diffraction pattern.  $\text{LiFePO}_4$  is the cathode material that the battery is composed of. LFP is a rechargeable battery composed of a natural mineral of the olivine family (magnesium iron silicate). This battery has a notably longer life cycle when compared to other lithium ions. Lithium actually is the lightest of the metal family as well and is also low maintenance which is a big advantage in terms of batteries. Although it has low electrical conductivity, it still has high performance and long-term stability. (Particle size was reduced to address this problem by covering the sample in conductive materials). The x-ray (AMPIX) cell is used to show the complex process that occurs in these operating batteries by consistently probing at fine reaction intervals. Argonne's AMPIX electrochemical cell is reliable over extended periods of time due to its uniform stack pressure, which is applied by x-ray windows.

## Motivation

Considering the rising use of batteries in modern technology, improved battery technology must be called for in order to enhance battery performance. Enhanced battery performance is mainly qualified by a battery's high power storage, voltage, discharge curve, capacity, energy density, and power density. Multiple methods are currently in practice to ensure the production of a high-performing battery that contains such qualities. Altering factors in battery manufacturing, specifically particle size of battery materials, produces batteries with varied efficiencies. Determining which particle and particle size produces the most efficient battery is crucial to improving battery technology. Experimenting with various cathode materials such as  $\text{LiFePO}_4$ ,  $\text{FePO}_4 \cdot x\text{H}_2\text{O}$ , and  $\text{FePO}_4 \cdot x\text{H}_8\text{O}$  will ensure the production of high-performing batteries.

## Experiment

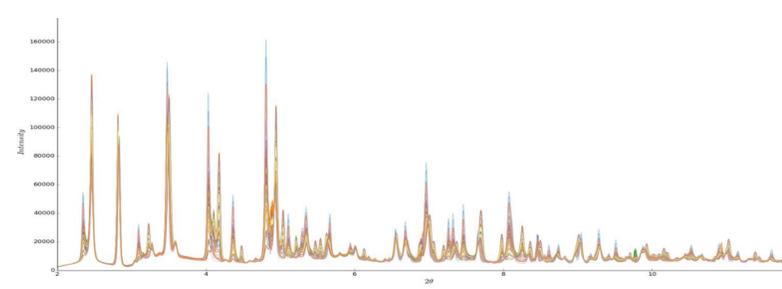


To determine whether or not initial material structure effects battery efficiency, samples of  $\text{LiFePO}_4$ ,  $\text{FePO}_4 \cdot x\text{H}_2\text{O}$ , and  $\text{FePO}_4 \cdot x\text{H}_8\text{O}$  were used in the preparation of the electrodes pellets. Mixtures of active material were mixed with graphite, carbon black, and PTFE binder in a mass ratio of 6:1:1:2. Mixtures were then transferred to a 10 mm diameter pressure die set, then pressed into pellets with thickness of 120-180  $\mu\text{m}$ . Electrode pellets were assembled into the electrochemical cell with a glass fiber separator (Whatman GF/A), Li- metal foil, and liquid electrolyte (1M LiPF6 in 1:1 v:v ethylene carbonate: dimethylcarbonate, EC:DMC) within an Ar-atmosphere glovebox.

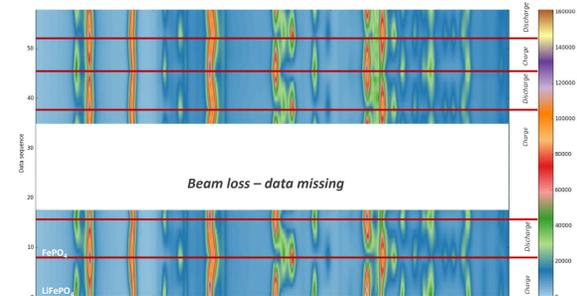
The cells were then cycled at a constant current of  $\sim 10$  mA/g at room temperature within the range 4.5mV-10mV. The rate at which batteries were cycled was determined through calculations of each sample's theoretical capacity (Q), actual capacity ( $C_p$ ). Through these calculations, the the calculated current (i) was determined using the equation ( $i = C_p / t$  [Ah/h]).

X-ray diffraction data were also collected at 30 minute intervals during the first discharge-charge cycle. High energy X-rays ( $\sim 58$  keV,  $\lambda = 0.2128$   $\text{\AA}$ ) as well as an amorphous-silicon based area detector were used for data extraction. GSASII was also used to reduce scattering images to one-dimensional data. X-ray data were collected at the 11-ID-B beamline at the Advanced Photon Source, Argonne National Laboratory.

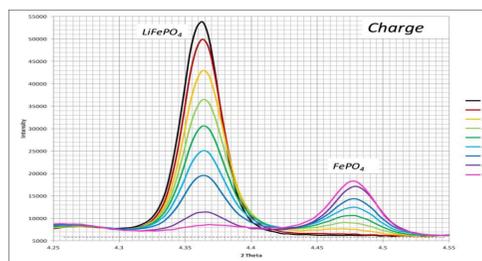
## Data



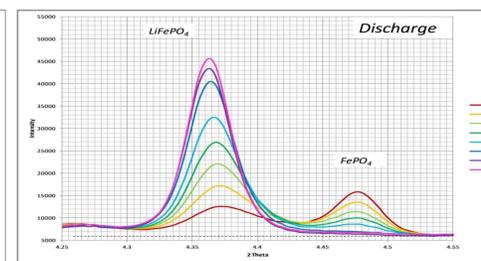
**Figure 1.** Structural changes within cathode material during battery operations



**Figure 2.** Top view at the peak positions and intensities changes during cycling. Initial material on the bottom of the graph. 3.5 cycles recorded. Beam was lost during data collection.



**Figure 3a.** Changes within peaks in area of interest while charging the  $\text{LiFePO}_4$  batteries



**Figure 3b.** Changes within peaks in area of interest while discharging the  $\text{LiFePO}_4$  batteries

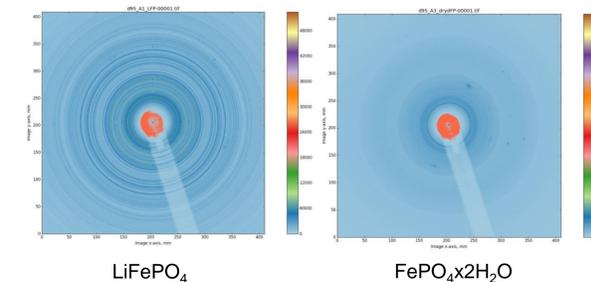
## Conclusion

After the conduction of the experiment, it can be concluded that the cathode materials with the unclear diffraction patterns (i.e.  $\text{FePO}_4 \cdot x\text{H}_2\text{O}$  and  $\text{FePO}_4 \cdot x\text{H}_8\text{O}$ ) are amorphous structures. Regarding electrochemistry, neither hydrated nor dehydrated  $\text{FePO}_4$  were able to be cycled at the desired speed. The material dried in the oven (dehydrated) was cycling only when slowed down 100 times. The other material (hydrated) always failed to be cycled. Consequently, no analysis in regards to the cycling of batteries was able to be generated for these two cathode materials.

In contrast, due to its diffraction pattern of multiple clear and well-defined rings, it can be concluded that the structure of  $\text{LiFePO}_4$  is crystalline. Electrochemically, this cathode material cycled the best. In contrast to the other two cathode materials, x-ray diffraction analysis was able to be collected and measured for the  $\text{LiFePO}_4$  battery. However, due to the lack of extended x-ray diffraction analysis for the other two materials, further comparison between cathode materials in regards to electrochemistry can not be made. Material optimization (especially in the cathode) is significant in developing battery technology in the future.

## Results

- $\text{LiFePO}_4$  sample was able to be cycled, and x-ray diffraction analysis was able to be generated.
- The other two cathode materials were not able to be cycled at the desired speed. No extended x-ray diffraction analysis was generated.
- The diffraction pattern of  $\text{LiFePO}_4$  displays clear rings upon measurement, a crystalline structure.
- The diffraction patterns in the other two cathode materials were unclear, with the exception of a few rings.



## Acknowledgements

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## References & Citations

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