

# Two-dimensional Model of a Lithium Iron-Phosphate Single Particle

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## Abstract

Introduction: Lithium-ion batteries are widely used as power sources for portable electronic devices (laptop, phones, and players) and electric cars due to their high energy density. New applications, such as Formula E, require also a huge power capability that the iron-phosphate-based positive electrode is able to provide. Indeed, a recent publication [1] shows that, at the particle level (20  $\mu\text{m}$ ), such a material is able to sustain a 4s-discharge (500C). The safety and sustainability of iron-phosphate makes it a good candidate for high-power storage application. The only drawback remains its lower energy density, compared to cobalt oxide or mixed oxide positive electrodes, due to a lower voltage. However, understanding how the power capability decreases during the scaling up of the electrode might help to improve even more the design and performance of this Li-ion technology.

Use of COMSOL Multiphysics®: The choice of COMSOL Multiphysics® software for the modeling of this single iron-phosphate particle came from the idea of demonstrating the lack of understanding of the fundamental phenomena that are at stake during the operation of insertion electrode materials. Of course, many models have been published so far in this field, but they all rely on the same set of PDEs [2]. In fact, using COMSOL makes it easy to implement new coupled PDEs and analytical expressions describing variable-dependent properties. Thanks to these features, we were able to show that the role of electrode kinetics has been widely underestimated, whereas diffusion of Li inside the particles has always been depicted as responsible of the limiting behavior of the Li-ion electrodes. The use of a 2D-axis symmetry geometry increases the computation time, without losing the possibility to show everything in 3D; COMSOL offers the possibility to reconstruct the 3D equivalent plot from the 2D solution in the "Results" tab.

Results: The 2D-model of a single particle offers the possibility to implement a state of the art expression for electrode kinetics based on a novel electrochemical phase-field model [3]. The latter was designed for nanoparticles and was not validated with experimental data. However, it is worth mentioning that at high rates there is no phase separation in  $\text{LiFePO}_4$  anymore. The original phase-field model has therefore been simplified in order to speed up the computation. As foreseen, the diffusion of lithium ion inside the iron phosphate can no longer be the only explanation to the decrease of the available capacity when the rate increases. The electrode kinetics plays also a major role as limiting phenomenon.

Conclusion: A multiphysics-based model is suitable to simulate the electrochemical behavior of a single particle of iron phosphate. It is the first time that such a model is validated with experimental data. However, the conclusion made by the team who built this high-level experiment might be slightly different from the new knowledge gained with this single particle model.

## Reference

- [1] H. Munakata et al. Evaluation of real performance of LiFePO<sub>4</sub> by using single particle technique. *J. Power Sources* 217, 444-448 (2012)
- [2] D.M. Bernardi, J.Y. Go. Analysis of pulse and relaxation behavior in lithium-ion batteries. *J. Power Sources* 196, 412-427 (2011)
- [3] P. Bai et al. Suppression of Phase Separation in LiFePO<sub>4</sub> Nanoparticles During Battery Discharge. *Nano Lett.* 11, 4890–4896 (2011)