

Electrode Performance and Phase Transition Mechanism of KFeSO_4F for K-Ion Batteries

Kei Kubota, Tomoaki Shimamura, and Shinichi Komaba

Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan

E-mail: komaba@rs.kagu.tus.ac.jp

Potassium-ion batteries (KIBs) have attracted much attention as high-voltage and high-power batteries due to the lower standard electrode potential of K^+/K in ester-based electrolyte and weaker solvation of K^+ ion compared to those of Li^+ ion [1, 2]. Recently, electrochemical and reversible K insertion/extraction into/from graphite has been reported by X. Ji and our groups [1, 3] and graphite is recognized as a promising candidate for the negative electrode material of KIBs. Now, high-energy positive electrode materials are required and developed in the world [4]. Polyanionic materials should be suitable for K insertion/extraction due to the rigid open framework and high working-voltage compared to layered transition metal oxides [5]. In this study, we have focused on orthorhombic KFeSO_4F (*o*- KFeSO_4F) showing high working-voltage [6]. The charge/discharge performances in K cells and the reaction mechanism are investigated.

o- KFeSO_4F synthesized delivers discharge capacity of ca. 115 mAh g^{-1} with average working-voltage of ca. 3.6 V in a K cell with 1 mol dm^{-3} $\text{KPF}_6/\text{EC}:\text{PC}(1:1 \text{ v/v})$ in the voltage range of 2.0 – 4.8 V. The capacity is relatively larger and polarization is smaller than those in the previous literature [5], which is probably due to difference of electrolyte solution. Capacity retention is, however, insufficient and ca. 73% after 40 cycles. Excellent cycle stability has been achieved by using highly concentrated KFSA/DME electrolyte. Phase transition of *o*- KFeSO_4F during charge/discharge in K cell is investigated by *operando* and synchrotron *ex-situ* XRD measurements and will be presented.

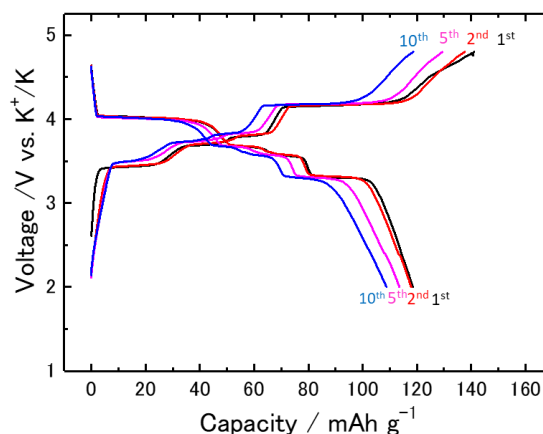


Fig. 1 Charge/discharge curves of *o*- KFeSO_4F in a K cell filled with 1 mol dm^{-3} $\text{KPF}_6/\text{EC}:\text{PC} (=1 : 1 \text{ v/v})$.

References:

- [1] S. Komaba, T. Hasegawa, M. Dahbi, and K. Kubota, *Electrochem. Commun.*, **60**, 172 (2015).
- [2] K. Kubota, S. Komaba, *et al.*, *Chem. Rec.* (2018), in press.
- [3] Z. Xing, X. Ji *et al.*, *J. Am. Chem. Soc.*, **137**, 11566 (2015).
- [4] K. Chihara, K. Kubota, S. Komaba *et al.*, *Chem. Commun.*, **53**, 5208 (2017).
- [5] Y. Hironaka, K. Kubota and S. Komaba, *Chem Commun.*, **53**, 3693 (2017).
- [6] N. Recham, J. M. Tarascon *et al.*, *Chem. Mater.*, **24**, 4363 (2012).