

# Study on improvement of cycle properties of TiS<sub>4</sub> positive electrode

Kentaro Kuratani<sup>a</sup>, Atsushi Sakuda<sup>b</sup>, Tomonari Takeuchi<sup>a</sup>, Hikari Sakaebe<sup>a</sup>,  
Hironori Kobayashi<sup>a</sup>

<sup>a</sup> National Institute for Advanced Industrial Science and Technology (AIST), 1-8-31,  
Midorigaoka, Ikeda, Osaka 563-8577 Japan

<sup>b</sup> Osaka Prefecture University, 1-1, Gakuen-cho, NakaKu, Sakai, Osaka 599-8531, Japan

E-mail: [k-kuratani@aist.go.jp](mailto:k-kuratani@aist.go.jp)

Sulfur (S) has attracted much attention as a positive electrode active material due to its high theoretical capacity (1672 mAh/g). On the other hand, sulfur includes some problems such as the dissolution of lithium polysulfide (Li<sub>2</sub>S<sub>x</sub>) into the electrolyte during charging and discharging. We have considered metal polysulfide is one of candidate materials for next generation lithium secondary batteries and reported novel metal polysulfides such as Li<sub>8</sub>FeS<sub>5</sub> [1], Li<sub>2</sub>TiS<sub>3</sub>, Li<sub>3</sub>NbS<sub>4</sub> [2, 3] and amorphous TiS<sub>4</sub> [4]. These materials can not only exhibit high capacity (over 600 mAh/g) but also suppress the dissolution of polysulfide by the formation of metal-sulfur bonds. The improvement of the capacity fading during cycling is, however, significant challenge to be solved for the practical use of metal polysulfides.

In this study, the capacity fading mechanism of TiS<sub>4</sub> was investigated by using charge-discharge measurement, X-ray absorption fine structure (XAFS) measurement, X-ray photo spectroscopy (XPS), and Raman spectroscopy.

We carried out the charge-discharge measurement of TiS<sub>4</sub> under three different temperatures (10 °C, 30 °C, 60 °C). The capacity fading caused by the film formation on the electrode and the dissolution of the redox species is, in general, accelerated as increasing the charge-discharge temperature. On the contrary, TiS<sub>4</sub> showed the similar cycle properties under above three temperatures. From this result, we consider the film formation and the dissolution of the redox species are not main reasons for the capacity fading of TiS<sub>4</sub>.

The application of electrolytes with high concentration successfully improved the cycle properties of TiS<sub>4</sub>. The capacity fading of TiS<sub>4</sub> was depressed with increasing the concentration of the electrolyte. The change of S K-edge spectra of TiS<sub>4</sub> implied that the reversibility of S was different between 3.5 M and 1.0 M. Detailed structural change of S during charging and discharging will be discussed in the poster.

## Acknowledgement

The authors would like to express thanks to Prof. T. Ohta and Dr. K. Nakanishi, Ritsumeikan University SR center, for their fruitful discussion of XAFS analysis.

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO) under the “Research and Development Initiative for Scientific Innovation of New Generation Batteries 2 (RISING2)”

## References:

- [1] T. Takeuchi, H. Kageyama, K. Nakanishi, M. Ogawa, T. Ohta, A. Sakuda, H. Sakaebe, H. Kobayashi, Z. Ogumi, *J. Electrochem. Soc.* 162 (9), (2015) A1745-A1750.
- [2] A. Sakuda, T. Takeuchi, K. Okamura, H. Kobayashi, H. Sakaebe, K. Tatsumi, Z. Ogumi, *Sci. Rep.* 4, Article No. 4883 (2014).
- [3] A. Sakuda, T. Takeuchi, H. Kobayashi, H. Sakaebe, K. Tatsumi, Z. Ogumi, *Electrochemistry*, 82, (2014) 880-883.
- [4] A. Sakuda, K. Ohara, K. Fukuda, K. Nakanishi, T. Kawaguchi, H. Arai, Y. Uchimoto, T. Ohta, E. Matsubara, Z. Ogumi, T. Okumura, H. Kobayashi, H. Kageyama, M. Shikano, H. Sakaebe, T. Takeuchi, *J. Am. Chem. Soc.*, 139 (2017) 8796-8799.