

Study of Sb and Sb-based Chalcogenide with Raman Spectroscopy, X-ray Diffraction and Dilatometry

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Sb is a promising anode material for lithium-ion battery for fast charging applications because of its suitable voltage range of about 0.8 V vs. Li/Li⁺ and higher capacity compared with commercial graphite. However, capacity of Sb decays significantly with cycling (see Fig. 1). In comparison, Sb-based chalcogenide material such as Sb₂Se₃ and Sb₂S₃, which undergo both conversion and alloying reactions, give better cycle performance when tested under the same conditions. We would therefore like to understand the role of S and Se in the charge-discharge mechanism of the materials.

In this study, we are conducting a comparison study between Sb, Sb₂Se₃ and Sb₂S₃ via several characterization methods including Raman spectroscopy, X-ray diffraction (XRD) and dilatometry at different state of charge or in-situ. XRD will enable us to monitor the change in crystallinity of the material during charge and discharge. Raman spectroscopy is a complementary method that can give us structural information even for amorphous materials. Dilatometry, in particular the measurement of the thickness change of the electrode during charge and discharge, can tell us the effect of the chalcogenide on the volume change during Li insertion and extraction. To eliminate particle size effect, Sb, Sb₂Se₃ and Sb₂S₃ with the same particle size are used. Combining these methods, we will be able to correlate their electrochemical performance with their chemical and mechanical properties. Results will be reported at the meeting.

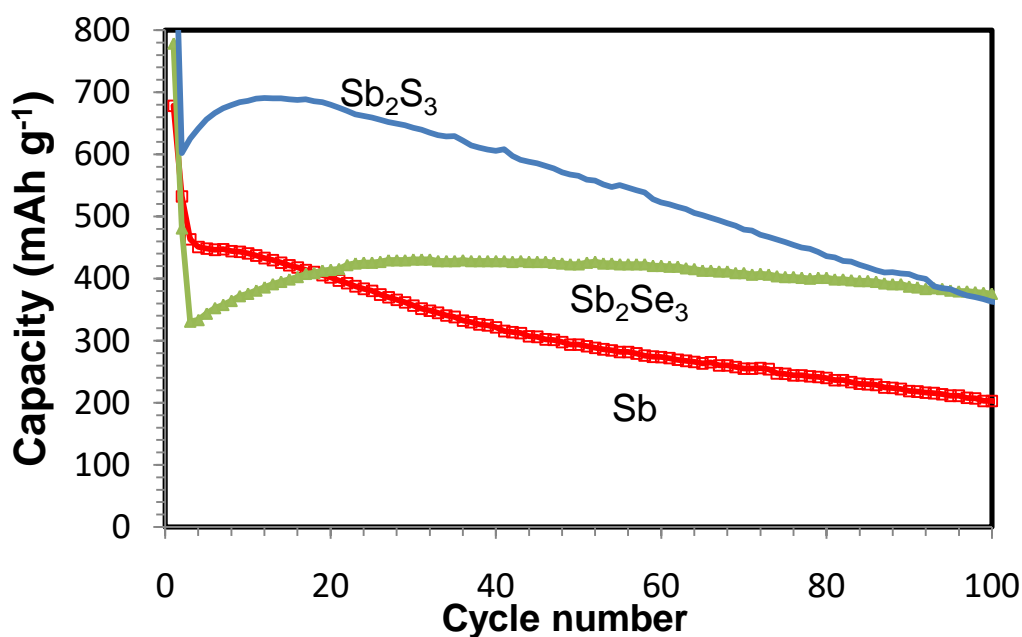


Figure 1. Cycle performance of Sb, Sb₂Se₃ and Sb₂S₃ with PAA as the binder