Titanium as Atomic Glue to Reduce Intrinsic Volume Expansion of Silicon during Li Alloying

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Silicon has been intensively investigated as a next-generation anode material for lithium-ion batteries (LIB) because of its high gravimetric capacity (3570 mAh g^{-1}) and a low lithiation voltage (0.4 V vs Li/Li^+). The major challenge of Si anode is its poor cycle stability due to drastic volume expansion of more than 300% when it alloys with lithium. Numerous methods such as the use of nanostructures, carbon coating, binder formulation, etc. have been investigated to increase the stability of Si electrodes by accommodating the volume change within the electrode and reducing particle fracturing. However, these methods do not alter the intrinsic lattice expansion within the Si material when Li is inserted. Here, we study the effect of Ti addition on the volume change of Si with Li alloying.

In order to eliminate the effect of the binder and porosity in the electrode, Si-Ti thin films with different amount of Ti (ranging from 43-100 at%) were made by RF magnetron sputter deposition (co-sputtering) under vacuum condition on copper foil. The thickness change of the electrode during lithiation and delithiation is monitored by an in-situ dilatometer with Li as counter electrode and 1M $LiPF_6$ in fluoroethylene carbonate (FEC) and diethyl carbonate (DEC) with a volume ratio 1:1 as the electrolyte. In addition, 2032 coin cells are made to investigate the cycle stability of the electrodes.

Fig. 1a shows a comparison of the thickness change of the Si and Si80-Ti20 electrode during 1st discharge. Even though Ti addition reduces the amount of Li that can be alloyed with Si, it acts as an atomic glue between Si atoms and reduces the volume expansion. Thickness change is only about 125% for Si80-Ti20 film after lithiation with 3 Li, half of that of Si film with the same amount of Li. With 20 at% Ti, the cycle performance of the electrode is significantly improved (Fig. 1b). More results on the Si-Ti thin films including full cell electrochemical tests and characterizations will be presented at the meeting.

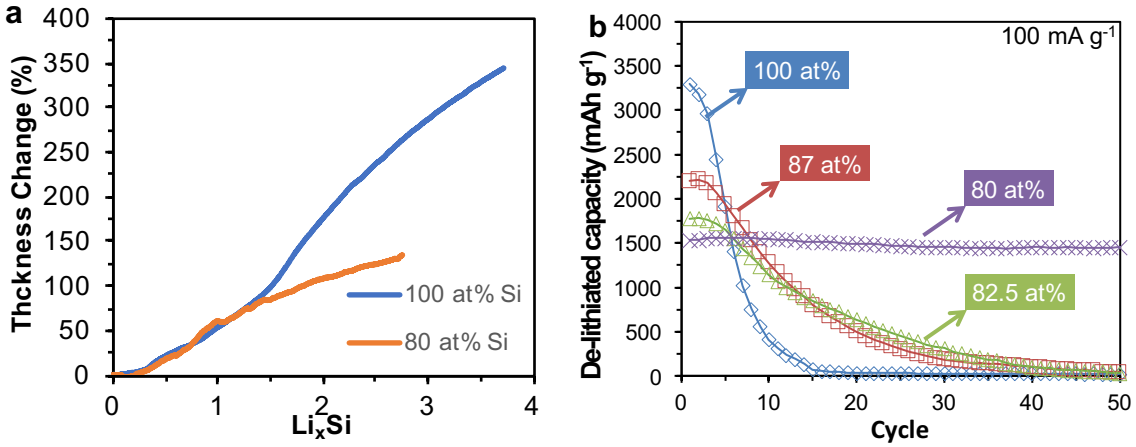

Fig. 1. (a) Electrode thickness change of Si and Si80-Ti20 electrodes during initial discharge. (b) Cycle performance of Si-Ti electrodes (percentage shown represents the amount of Si in the film).