In situ Study of Silicon-Based Thin Film Anodes for Lithium Ion Battery

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Silicon (Si) has become a forefront candidate among other anode materials suitable for high-performance lithium-ion batteries (LIBs)[1]. The interest of scientists is caused by its high specific capacity of 3579 mAh g^{-1} achievable upon formation of the $Li_{15}Si_4$ silicide, a theoretical volumetric capacity of 2190 mAh cm^{-3}, a comparatively low discharge potential of 0.4 V vs. Li/Li^+, and low cost and safety[2,3]. However, an alloying nature of Si lithiation, which leads to a high capacity, is inevitably accompanied by an undesirable volume expansion. The latter calls a strain stress arising in the Si material bulk that, upon repeated cycling, leads to its mechanical degradation, pulverization, electrical contact loss leading to capacity loss and even to safety issues[4].

There are several silicides like $Li_{12}Si_7$, Li_7Si_3, $Li_{13}Si_4$, $Li_{15}Si_4$, $Li_{21}Si_5$, $Li_{17}Si_4$, $Li_{22}Si_5$ which can form at the Si and Li interaction depending on conditions. Despite, $Li1_5Si_4$ acts as the highest lithiated phase, which forms below the potential of 50 mV at room temperature [5], it is interesting to know a crystallization mechanism of the lithiuim silicides with the higher lithiation form usually which usually forms at the prolonged lithiation at 0 V[6]. Thus, this work reports the results of a in situ Raman spectroscopic investigation of electrode during lithiation/delithiation. The details of the research will be presented at the conference.

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