Li-Si Alloy Anode for the Li Rechargeable Batteries

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The state of art technology in the rechargeable batteries use the $LiCoO_2$ cathode, graphite anode and anhydrous electrolyte. Although graphite anode provides high energy density and low cost, they have limited specific capacity of around 360mAh/g and low volumetric energy density. Thus, various anode materials have been investigated to replace for the graphite anode. Si has gained attention due to the large specific capacity and volumetric capacity. One mol of Si can take up 4.4 mol of Li into the structure forming $SiLi_{4.4}$, which corresponds to the capacity of 4000 mAh/g. However, Si powder undergoes large volume change during the Li insertion and extraction, resulting in the capacity fade. To overcome the mechanical failure, various methods have been proposed including ternary intermetallic compounds and amorphous Si oxides.

The Li-Si systems exhibit a various phases, i.e., LiSi, $Li_{12}Si_7$, $Li_{14}Si_6$, $Li_{13}Si_4$, and $Li_{22}Si_4$ in the phase diagram. Li was shown to diffuse rapidly in the Li-Si system. Knowledge concerning the structure of each phases is crucial to understanding the charging and discharging behavior of Si anode. In this study, we will present the ^{6}Li and ^{29}Si MAS NMR results of Si anode at various status of charging. Several ^{6}Li resonances were observed as the extent of charging increases, indicating the various (local) structure for the Li. In contrast, no significant change in the Si shift was seen, suggesting a very weak bonding between Si-Li. The information from this study will be used as a fingerprint to analyze the more complicated system such as a ternary silicide(e.g. M-Si-Li).

References

[1] H. Li, X. Huang, L. Chen, G. Zhou, Z. Zhang, D. Yu, Y. J. Mo. N. Pei, *Solid State Ionics*., **135**, 181 (2000).
[2] C. J. Wen, R. A. Huggins, *J Solid State Chem*,.**37**, 271 (1981).
[3] L.A. Stearns, J. Gryko, J. Diefenbacher, G. K. Ramachandran, P. F. McMillan, *J. Solid State Chem*, **173**, 251 (2003).

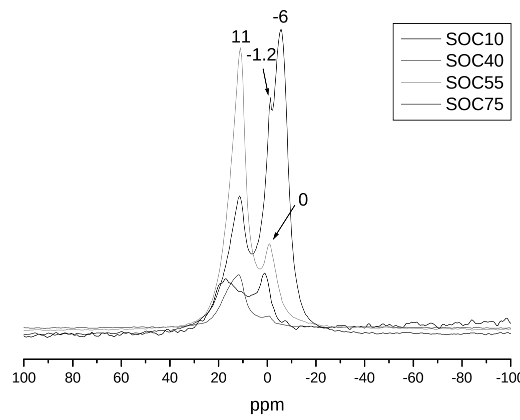

Fig. 1. ^{6}Li MAS NMR spectra of Li-Si anode at various status of charging.

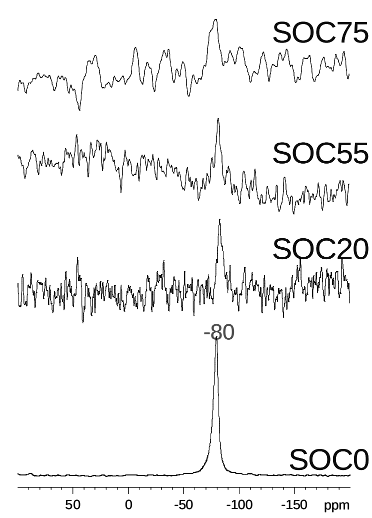

Fig. 2. ^{29}Si MAS NMR of Li-Si anode

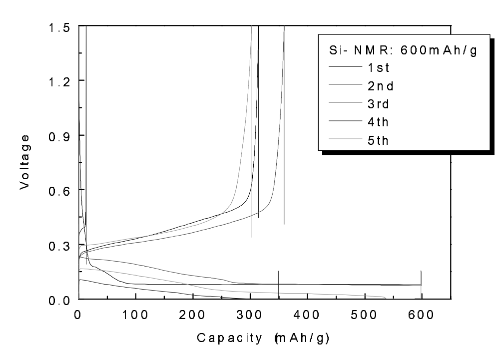

Fig. 3. Potential profile of Li-Si anode