

# Improved performances of amorphous Si electrodes by incorporation of methyl groups



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Silicon is one of the most attractive anode materials for Li-ion batteries due to its high theoretical charge capacity,  $3579 \text{ mAh g}^{-1}$ . The main limitation of this material is the very large volume expansion accompanying incorporation of Li ions. Using silicon in nanoscale form (thin films, powders, nanowires...) is considered as the most promising strategy for overcoming this limitation. The use of heterogeneous mixtures of carbon and silicon grains also improves the cycling properties of silicon. However, even in such mixtures, volume changes during lithiation/delithiation cycles remain an important issue.

We recently reported [1] that amorphous thin films of silicon-carbon alloys prepared by low-power Plasma Enhanced Chemical Vapor Deposition (PECVD) exhibit significantly improved performances. In these films carbon is mostly inserted as methyl groups, forming the compound  $a\text{-Si}_{1-x}(\text{CH}_3)_x\text{H}$ , where  $x$  may be tuned continuously between 0 and 0.4.

We report here a systematic study of the evolution of these films during lithiation/delithiation cycles. Several techniques were used, including Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR). Morphological changes of the films were followed by in-situ imaging and characterized quantitatively by ex-situ noncontact Atomic Force Microscopy (nc-AFM).

[1] L. Touahir, A. Cheriet, D. Alves Dalla Corte, J.-N. Chazalviel, C. Henry de Villeneuve, F. Ozanam, I. Solomon, A. Keffous, N. Gabouze, M. Rosso, *J. Power Sources* 240 (2013) 551-557