

# Si-Fe-based Alloy Negative Electrode Materials with Extraordinary High Thermal Stability

Yijia Liu<sup>a</sup>, Michael A. Charlton<sup>a</sup>, M.N. Obrovac<sup>b</sup>

<sup>a</sup>Department of Chemistry, Dalhousie University,

<sup>b</sup>Department of Physics and Atmospheric Science, Dalhousie University, Halifax, NS, B3H 4R2

E-mail: YijiaLiu@dal.ca

Nanostructured Si-Fe-based alloys for high energy density Li-ion negative electrodes were prepared with a unique microstructure with extraordinary high thermal stability. Excellent cycling characteristics were maintained, even after annealing the alloys to 800°C. This temperature stability far surpasses conventional Si-Fe or other Si-M alloys, which typically lose significant capacity and crystallize when heated near 600°C.

Conventional Si-Fe alloys severely crystallize when heated near or above 600°C, resulting in the formation of  $\text{Li}_{15}\text{Si}_4$  during cycling, as shown in Figure 1(a). However, the present Si-Fe-based alloys were found to be remarkably thermally stable. These Si-Fe-based alloys exhibit voltage profiles that are characteristic of amorphous Si. No  $\text{Li}_{15}\text{Si}_4$  formation was observed and excellent cycle life could be maintained, even after heating to 800°C, as shown in Figure 1(b). In fact, the cycle life of the present alloys improved after heating to 600°C or 800°C, while having a high reversible volumetric capacity of 1500 Ah/L.

The thermal stability of the present alloys is an important advance in alloy electrode materials. The ability of these alloys to maintain stability at high temperatures makes them amenable towards high temperature processing, including carbon coating, allowing for further improvements in cycling stability. In this presentation the methods to obtain high thermal stability in alloys will be explained and their special microstructure will be described.

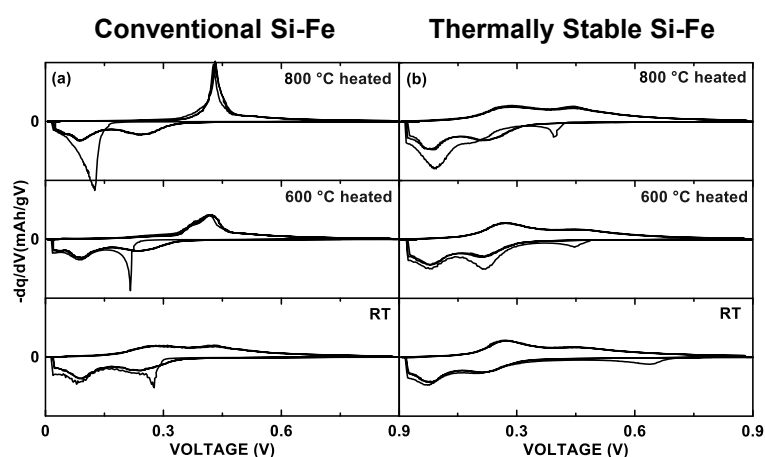


Figure 1: Differential capacity curves of (a) a conventional Si-Fe alloy and (b) a thermally stable Si-Fe-based alloy.

## References:

- [1] A.M. Wilson, J.R. Dahn, J. Electrochem. Soc. 142 (1995) 326.
- [2] M.N. Obrovac, V.L. Chevrier, Chem. Rev. 114 (2014) 11444–11502.