Si-Ti-N Alloy Negative Electrodes with Extremely High Thermal Stability for Li-Ion Batteries

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Si-Ti-N alloys are conventionally made by ball milling Si and TiN. We have found that such conventionally ball milled alloys crystallize during heating. Using a new method we prepared Si-Ti-N alloys with a unique microstructure allowing for high temperature thermal processing. X-ray diffraction patterns of thermally stable (TS) $Si_{70}Ti_{30}N_{30}$ and of the same sample heated to 800°C are shown in Figure 1. The XRD patterns are similar and are mainly made up of amorphous Si and nanocrystalline TiN. In contrast, conventional ball milled Si + TiN, underwent severe crystallization at 800°C (also shown in Figure 1).

The new thermally stable Si-Ti-N alloys are also more structurally stable during cycling and maintain their structural integrity even after heating to thigh temperatures. High temperature tolerance enables TS-Si-Ti-N alloys to be carbon coated at high temperature, which is an important method to improve performance of Si alloy electrode materials.

The microstructure, thermal stability and cell performance of TS-Si-Ti-N alloys with different stoichiometry will be presented, and reasons for their improved temperature tolerance will be discussed.

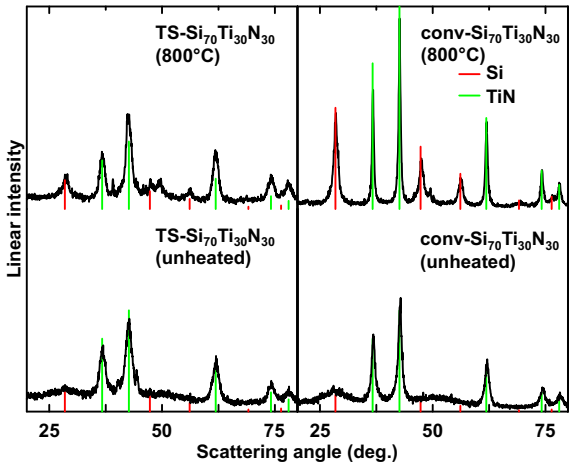

Figure 1 XRD patterns for unheated and heated TS-$Si_{70}Ti_{30}N_{30}$ conventional $Si_{70}Ti_{30}N_{30}$ samples.