Abstract

In order to fully understand the transition mechanism of a processed thermal battery, X-ray Diffraction and X-ray Fluorescence were employed to characterize various quench states. The transition of interest in this report is the formation of Li_7Si_3 from $Li_{13}Si_4$ (initial Anode material). The unit cell conditions during $Li_{13}Si_4$ transition to Li_7Si_3 show a contraction of 0.04 and 0.02Å (a and b-axis respectively), an expansion in the c-axis of 0.02Å, and an overall reduction in the cell volume from 541.13 $Å^3$ to 539.21$Å^3$ for the $Li_{13}Si_4$ Orthorhombic (Pbam) component. The contraction in the a-b plane results from the loss of Li atoms; the expansion in the c-axis direction is due to reorganization of the Li and Si within the unit cell. Transition processing also requires that an excess of 3⅔ moles Li (within Anode region) react with S (within Cathode region) to form Li_2S. X-ray Fluorescence confirms a definite migration of S through the Separator region during the transition. These results both explain peak shifts (in Anode regions) and the formation of Li_2S during transition states.