Ball Milling Kinetics, Microstructure and Performance of Si-M (Fe, Cr, V) Alloys

Benjamin Scott [a], Clarke Brown[a], M.N. Obrovac [a,b]
[a] *Dalhousie University Department of Chemistry, Halifax, NS B3H 4R2, Canada*
[b] *Dalhousie University Department of Physics and Atmospheric Science, Halifax, NS B3H 4R2, Canada*
E-mail: B.Scott@dal.ca

Si-M (M = transition metal) alloy negative electrodes for Li-ion batteries have garnered considerable research interest because of its high volumetric capacity, thermal stability, and relatively low cost. However, little attention has been paid to the role of the inactive phase in determining the ease of synthesis, final microstructure, and ultimate performance of these alloys.

In this work $Si_{85}TM_{15}$ (TM = Fe, Cr, V) alloys were prepared by mechanical alloying (MA). Relative MA reaction rates were observed via X-ray diffraction (XRD) and Mössbauer spectroscopy. The MA rate and ultimate microstructure was found to be dependent upon the inherent mechanical properties of that transition metal, as shown in Figure 1. Time to reach steady state and final grain size varied significantly depending on the transition metal used. Cycling performance was also found to be dependent on the transition metal used. This work highlights that although the transition metal and transition metal silicide are inactive during lithiation; the choice of transition metal plays a significant role in the mechanochemical reaction and ultimately electrochemical performance.

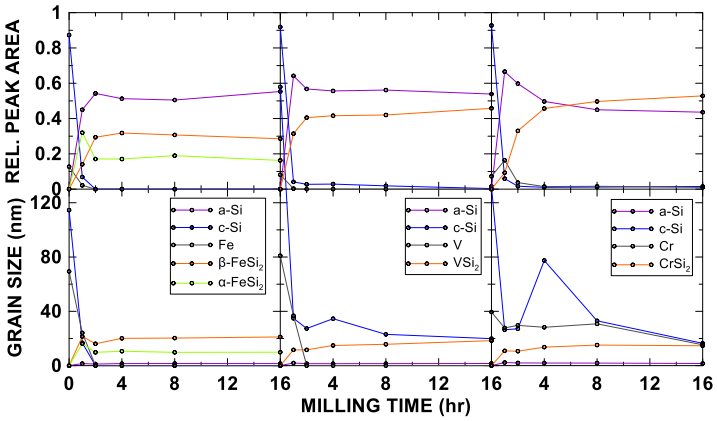

Figure 1 Trends in relative XRD peak area and grain size of each phase during the mechanical alloying of $Si_{85}TM_{15}$ (TM = Fe, Cr, V) alloys.

References:

[1]. M. N. Obrovac, L. Christensen, D. B. Le, and J. R. Dahn, J. Electrochem. Soc. 154 (2007) A849.
[2]. M. N. Obrovac and L. Christensen, Electrochem. Solid-State Lett. 7 (2004) A93.