

Studies of Si-Fe-C Electrode Materials Prepared By Combinatorial Sputter Deposition

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Combinatorial studies of Si-Fe-C system are presented. The structure of the resulting thin films was studied using X-ray diffraction (XRD). Mössbauer spectroscopy was employed to study the atomic environment. Cyclic voltammetry measurements were performed to study the behavior of these materials as negative electrodes for Li-ion batteries [1].

Figure 1 shows the Gibbs' triangle for the Si-Fe-C library and illustrates the compositions of the sputtered library.

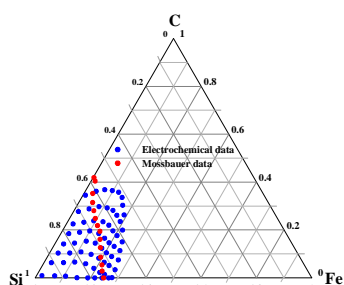


Figure 1 Gibbs' triangle for the Si-Fe-C system showing compositions of the $\text{Si}_{1-x-y}\text{Fe}_x\text{C}_y$ library as determined by electron microprobe analysis.

XRD patterns (not shown) show that a substantial portion of the compositions prepared in this work are amorphous or nanostructured and, from a structural standpoint, show potential for use as electrode materials.

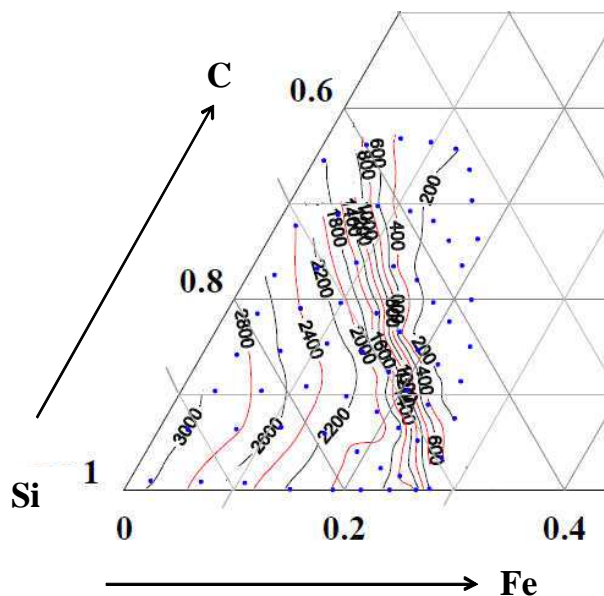


Figure 2: 1st delithiation capacity (mAh/g) as a function of composition for Si-Fe-C. Dots indicate compositions used to produce the contours.

Figure 2 shows the first delithiation capacity (mAh/g) from the sputtered electrodes. As shown in this figure, the capacity diminishes as the amount of iron increases.

Figure 3 shows differential capacity curves for selected compositions. These plots show fairly broad features, with no changes in their overall shape during cycling. This may indicate that no major changes occur in the structure of the materials upon cycling. More details on the electrochemical performance will be presented.

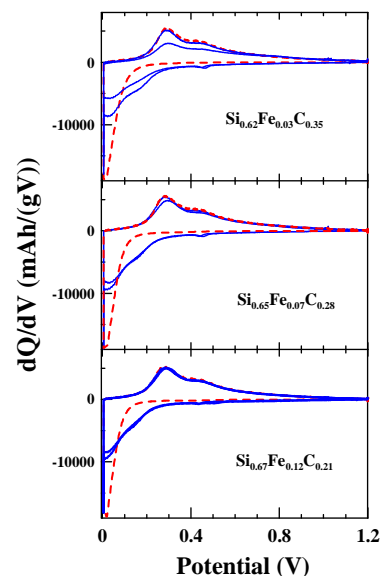


Figure 3: dQ/dV vs. V plots for the first three cycles; dashed (red) line for first cycle, continuous (blue) line for second and third cycles. The compositions are indicated.

Figure 4 shows selected Mössbauer spectra. Mössbauer spectra were fit to a Voigt-based function (VBF), as described in [2], corresponding to a single Gaussian distribution of symmetric quadrupole split doublets, as is appropriate for such materials. More detailed analysis will be presented.

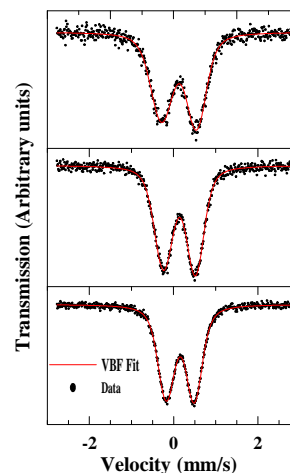


Figure 4: Selected room temperature ^{57}Fe Mössbauer effect spectra of samples from pseudobinary library (shown in Figure 1); experimental data (circles) and VBF fits (solid lines).

References

- [1] M. D. Fleischauer, T. D. Hatchard, G.P. Rockwell, J.M. Topple, S. Trussler, S.K. Jericho, M. H. Jericho and J.R. Dahn, *J. Electrochem. Soc.* 150, A1465 (2003).
- [2] D. G. Rancourt and J. Y. Ping, *Nucl. Instrum. Meth.* 97, B58 (1991).

