Electrochemical Properties of Ternary Si-A-B Alloy Negatives for Li-ion Batteries.

T.D. Hatchard and J.R. Dahn Dept. of Physics, Dalhousie University, Halifax, Nova Scotia, B3H 3J5, Canada

With the continuing miniaturisation of electronic devices such as cell phones and PDAs, the demands put on rechargeable batteries are being pushed ever higher. As a result, research efforts to find better electrode materials have been focusing on a broad range of materials. An attractive possibility for negative materials is Si-based alloys, with much work being done to improve their performance in Li-ion cells [1].

Using the methods of combinatorial materials science [2], a single film can be made in a matter of hours which contains a range of stoichiometries. Using the combinatorial materials science infrastructure that we have built at Dalhousie [3 - 5], ternary films can be made consisting of Si-A-B alloys, where A,B = Group IV or transition metal. 75 mm x 75 mm wafers are made where the silicon content is kept fixed and elements A and B vary linearly and orthogonaly to one another. The films are characterized in terms of structure and composition, and then tested for electrochemical performance in a 64 channel combinatorial test cell. Figure 1 shows an example of a non-equilibrium ternary phase diagram (Gibb's Triangle) constructed for one ternary system (Si-Ag-Sn).



Figure 1. Non-equilibrium ternary phase diagram for sputtered films in the Si-Ag-Sn ternary system.



Figure 2. Sample of dQ/dV versus V for Si-Ag-Sn.

This talk will summarize electrochemical results for several Si-A-B ternary systems. Data to be included will be dQ/dV versus V and potential versus specific capacity. Also, the approximate amorphous ranges in the as-sputtered materials will be reported, as this is of importance to the electrochemical cycling of the material. Figure 2 shows an example of dQ/dV versus V data for a Si-Ag-Sn ternary film collected with a 64-channel combinatorial electrochemical cell. Figure 3 shows



potential versus specific capacity for the same film.

Figure 3. Potential versus specific capacity data for Si-Ag-Sn.

References.

[1] Good review articles: M. Winter and J.O. Besenhard, Electrochimica Acta, 45, 31-50 (1999). R.A. Huggins in: J.O. Besenhard (Ed.) Handbook of Battery Materials,

Wiley-VCH. Weinheim, 1999, Part III, ch. 5.

[2] X. D. Xiang, et. al., A Combinatorial Approach to Materials Discovery, Science, 268 p1738, 1995.

[3] J.R. Dahn, S. Trussler, T.D. Hatchard, A.

Bonakdarpour, J.R. Mueller-Neuhaus, K.C. Hewitt and M.D. Fleischauer, Chemistry of Materials, 14(8), 3519-3523, 2002.

[4] M.D. Fleischauer, T.D. Hatchard, G.P. Rockwell, J.M. Topple, S. Trussler and J.R. Dahn, J. Electrochem. Soc. 150 (11) A1465-A1469 (2003).

[5] Vivien K. Cumyn, M.D. Fleischauer, T.D. Hatchard and J.R. Dahn, Electrochem. Solid State Lett. 6 (2003) E15.