

### Structural and Electrochemical Properties of SiM Binary Alloys.

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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].

Although many materials being studied for use as electrode materials contain multiple elements, it can be more instructive to study a simpler system. Many negative materials for Li-ion cells being studied are Si based alloy materials. To learn more about how these materials will behave when alloyed with Li, some Si-M binaries have been produced where M = Group IV or transition metal elements (these elements are commonly alloyed with Si in negative materials [2]).

Using the methods of combinatorial materials science [3], 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 [4 - 6], a binary film can be produced and analysed very rapidly. 75 mm x 75 mm wafers are used as substrates upon which the silicon content is kept fixed and element M is varied linearly in one direction. The films are characterized in terms of structure and composition, and then tested for electrochemical performance in a combinatorial test cell. Figure 1 shows an example of Sn:Si (at%) ratio for a binary film. The contours are superimposed on a combinatorial cell plate [5] used to test the electrochemical properties of the film.

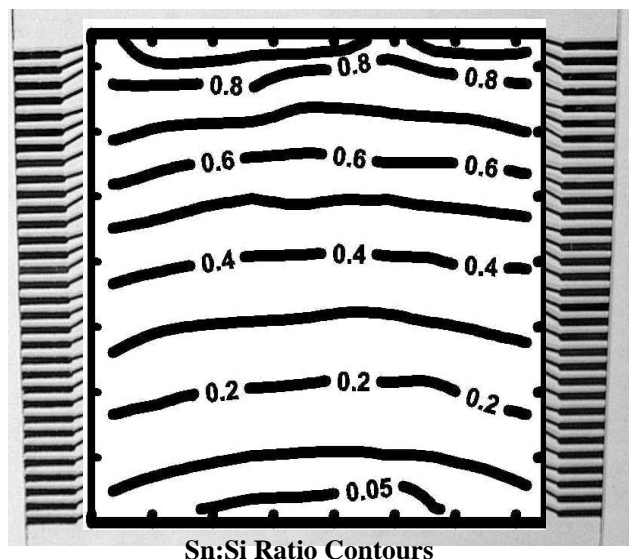
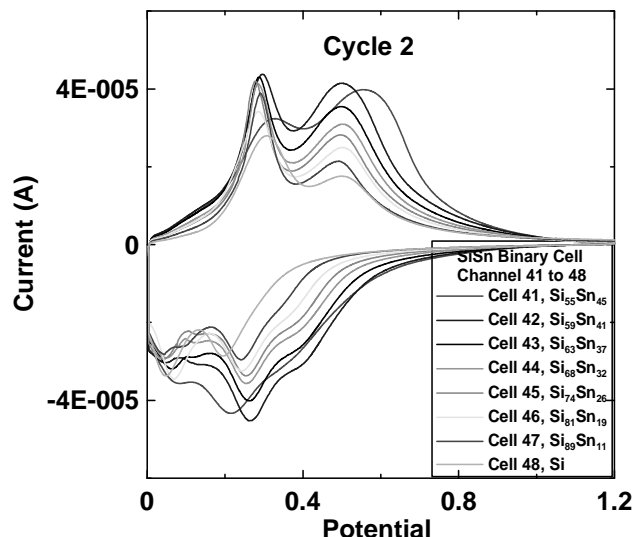


Figure 1. Combinatorial cell plate with Sn:Si ratio contours superimposed.

Using this method, it is very easy to determine the



effects of adding element M to a-Si. Figure 2 shows a series of I versus V data for one column of the combinatorial cell plate with the Si-Sn film sputtered on it. It can be seen that adding just a small amount of Sn to a-Si has significant effects on the shape of the I versus V curve.

This talk will present the results of studies performed on various Si-M binary systems. The effects on electrochemical performance of adding these elements to a-Si will be summarized.

Figure 2. I vs. V for one column of channels from the Si-Sn binary combinatorial cell plate.

### 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] T.D. Hatchard and J.R. Dahn, Electrochemical properties of ternary alloy negatives for Li-ion batteries, abstract submitted to this meeting.
- [3] X. D. Xiang, et. al, *Science*, **268** p1738, 1995.
- [4] 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.
- [5] 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).
- [6] Vivien K. Cumyn, M.D. Fleischauer, T.D. Hatchard and J.R. Dahn, *Electrochem. Solid State Lett.* 6 (2003) E15.