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

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 orthogonally 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).

![Non-equilibrium ternary phase diagram for sputtered films in the Si-Ag-Sn ternary system.](image)

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

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.

![Sample of dQ/dV versus V for Si-Ag-Sn.](image)

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

References.