

## AuNi<sub>2</sub>Sn<sub>4</sub> with R3m Space Group as a Model for Ternary Alloy Anodes for Rechargeable Lithium Batteries

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There has long been a search for intermetallic alloy materials to serve as anodes in lithium batteries. These alloys have high volumetric and gravimetric lithium storage capacities compared with current carbonaceous anodes. The AuNi<sub>2</sub>Sn<sub>4</sub> alloy, which is rich in lithium alloying elements such as Sn, has the proper coordination and spacing to absorb large amount of lithium with a minimum volume change.

The ternary intermetallic AuNi<sub>2</sub>Sn<sub>4</sub> phase has been prepared by melting together stoichiometric amounts of the pure elements in a quartz glass tube, followed by annealing for 4 days at 400°C. Coatings for electrochemical cells were made by mixing together weighed amounts of finely ground sample, Shawinigan Black carbon and a binder dissolved in xylene. The coatings were made on a carbon coated Cu-foil. Electrochemical testing was performed using a battery setup against Li and with 1 M LiPF<sub>6</sub> in 1:1 DMC/EC as electrolyte. AuNi<sub>2</sub>Sn<sub>4</sub> shows a high lithium storage capacity of 1422 mAh/g in its initial discharge (Fig. 1). The initial discharge goes through two distinct steps, where the second step has the largest capacity for lithium ions. The subsequent charging of the material shows that only a fraction of this capacity is reversible (319 mAh/g), when charging up to 1.5 V. This cut off voltage is seen to be too low to access the second step in the discharge curve, and thus a higher cut off voltage was tested (Fig. 2). Indeed, then the reversible capacity upon discharge was 898 mAh/g. X-ray diffraction of the AuNi<sub>2</sub>Sn<sub>4</sub> phase indicates a negligible volume expansion as a result of lithium insertion. This may be explained by the ordered vacancies on every fourth layer in this structure, and also the size of the lithium ions. Cycling of this material has so far not been very successful, and it seems that despite small volume changes in the material, the grain size and contact with the current collector cause a very rapid degradation of the anode.

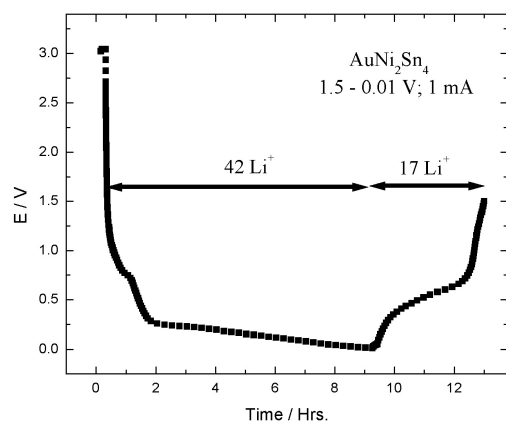


Fig. 1. First charge/discharge cycle of AuNi<sub>2</sub>Sn<sub>4</sub>, charging to 0.01 V and discharging to 1.5 V at 1 mA constant current conditions.

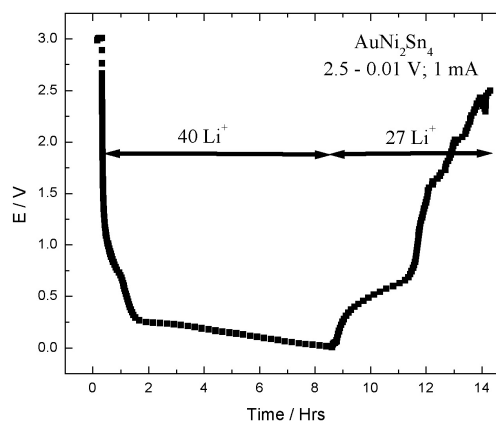


Fig. 2. First charge/discharge cycle of AuNi<sub>2</sub>Sn<sub>4</sub>, charging to 0.01 V and discharging to 2.5 V at 1 mA constant current conditions.