INTERMETALLIC INSERTION ANODES
FOR LITHIUM BATTERIES

by

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This work was performed under the auspices of the Office of Basic
Energy Sciences; Division of Chemical Sciences, U.S. Department

July, 1999

For presentation at the 196th Joint International of the Electrochemical Society,
Honolulu, Hawaii, October 17-22, 1999
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Intermetallic alloys have been investigated for many years as anode materials for lithium batteries and, more recently, as alternative electrodes to carbon, because of several intrinsic advantages including high capacity and safety (1,2). Some of the most studied alloys utilize tin as the active component because of its high theoretical capacity (996 mAh/g) and its slightly higher operating voltage (<400 mV) compared to metallic lithium (3). To date, the use of binary lithium alloys as anodes has been limited to the select number of main group elements (e.g. Sn) that can be lithiated at an appropriate voltage with acceptable kinetics. A major disadvantage of binary LiₓM alloy systems is that major phase changes occur during the electrochemical cycling of lithium. Severe volume expansion and contraction of the metal matrix, which limit the cycle life of the lithium cell, normally accompany these phase changes. The most successful approach to overcoming this limitation has been the use of intermetallic alloys MM' consisting of two (or more) metals, at least one of which is an “active” alloying element (M) and the other an “inactive” (M') element (4,5,6). During the reaction with lithium, such a system breaks up into regions of LiₓM and inactive M'. In our work, we have extended the concept of intermetallic electrodes to include topotactic reactions in which the intermetallic compound provides a host structure for lithium.

For instance, we have shown by in-situ X-ray diffraction that in the copper-tin system (Fig. 1), the following reaction takes place:

$$\text{Cu}_6\text{Sn}_5 + 13\text{Li} \leftrightarrow \text{Li}_{13}\text{Cu}_6\text{Sn}_5$$

In these types of reactions, the classic limitations of intermetallic anodes, such as volume expansion, can be reduced. This presentation will include our recent results on the copper-tin system and on related materials.

Figure 1. Structure of Cu₆Sn₅. Black spheres represent tin atoms; gray spheres represent copper atoms.