

## Characterization of the C-Zn System for Use in Lithium-Ion Batteries as Alloy Anode Materials

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### Introduction

Metal alloy negative electrode materials have significantly larger volumetric and specific energy density compared to conventional graphitic anodes in Li-ion batteries. Sn-Co-C based alloys have been utilized in commercial cells by Sony [1]. Studies of these alloys have shown that the carbon phase forms  $\text{LiC}_2$  during lithiation [2], corresponding to a volumetric capacity of about 1360 Ah/L, which is greater than twice the volumetric capacity of graphite. Alloys based on this form of carbon could potentially use low cost raw materials and have high capacities.

Here we investigate the complete Zn-C binary system for use as alloy materials in lithium ion batteries.

### Experimental

Thin film samples were synthesized through combinatorial sputtering using a modified Corona Vacuum Coaters V-3T deposition system equipped with a 500 L/s turbo pump and a Polycold system. Cu discs (1.91  $\text{cm}^2$ ) were sputtered onto directly and built into coin cells in an Ar-filled glovebox using 1 M  $\text{LiPF}_6$  in FEC/EC/DEC (1/3/6 by volume). X-ray diffraction (XRD) measurements of the thin films were performed using a Bruker AXS D8 Discover XRD system equipped with a copper target, an incident beam monochromator and an area detector. Electron microprobe measurements of the thin films were performed using a fully automated JEOL JXA-8200 Superprobe with a 50  $\mu\text{m}$  electron beam diameter at 50 nA and 5keV. Electrochemical cycling was performed using a Maccor Series 4000 Automated Test System at 30°C between voltage ranges of 1 mV to 1.5 mV and 1 mV to 2.5 V at a C/10 rate.

### Results

Figure 1 shows XRD patterns of alloys in the  $\text{Zn}_{1-x}\text{C}_x$  series. Compositions with high carbon content were amorphous, while compositions with high zinc content comprised crystalline Zn. Compositions in the range  $0.34 < x < 0.43$  were highly susceptible to air oxidation, forming ZnO.

Figure 2 shows voltage profiles of selected sputtered compositions. Oxygen content as determined by electron microprobe measurement are indicated. Plateaus indicative of 2-phase regions in the Zn-Li phase system progressively disappear as carbon is added and the alloy becomes nanostructured.

Figure 3 shows the delithiation capacity as a function of cycle number for alloys in this series. Alloys containing crystalline Zn suffered from severe capacity fade. Compositions with greater than 14% carbon content had good cycle life. Increasing the carbon content further lead to increased capacity.

The effects of composition on the crystal structure, irreversible capacity, coulombic efficiency and capacity retention of C-Zn alloys will be discussed.

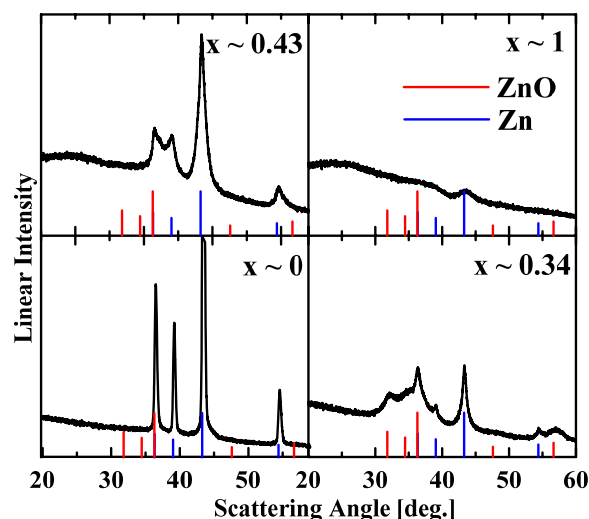


Figure 1

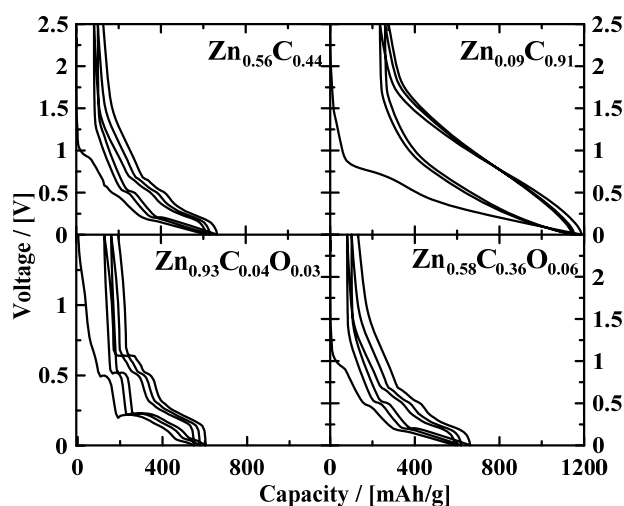


Figure 2

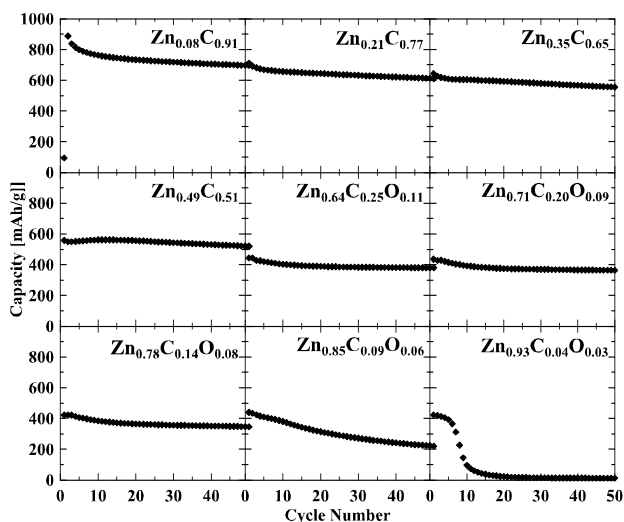


Figure 3

### References

- [1] <http://www.sony.net/SonyInfo/News/Press/200502/05-006E/>. Accessed July 2012.
- [2] J.R. Dahn, R.E. Mar and Alyaa Abouzeid, J. Electrochem. Soc. **153**, A361 (2006).