Synthesis and Structure of Conducting Polymers

Description: The Conducting Polymer Group applies an interdisciplinary approach to the synthesis and characterization of ion conducting polymers. The focus of the program is on ion-ion and ion-polymer interactions. Recent emphasis is on enhancing conductivity of polymer electrolytes by modifying the chemistry to increase the number of charge carriers and the Li' ion transference number. This is done by use of complexing polar plasticizers and anion complexing agents, and is coupled with the use of a wide array of spectroscopic techniques, such as x-ray absorption spectroscopy (XAS), to elucidate ion-ion and ion-polymer interactions and the conductivity mechanisms. The program involves synthesis and characterization work. There are two CRADAs. One with Power Conversion, Inc. of Elmwood Park, NJ to apply the BNL technology to thin film primary lithium batteries for use in electronic circuitry. The other is with Gould, Inc. of Cleveland, OH on additives for liquid non-aqueous electrolytes and characterization of battery cathode materials by in situ x-ray diffraction (XRD) and XAS.

Program Highlights:

The work on anion complexing agents has resulted in the synthesis of two new families of neutral anion complexing agents. One is based on electron deficient nitrogen sites on substituted aza-ethers, wherein the hydrogen on the nitrogen is replaced by electron withdrawing groups such as CF3SO3_- The other is based on electron deficient boron sites on borane or borate compounds with various fluorinated aryl or alkyl groups. A polymer electrolyte, based on the complexing of anions, was synthesized by grafting the aza anion acceptors onto a siloxane polymer backbone. The polymer can dissolve lithium salts such as LiCl to yield a new type of polymer electrolyte that contains no ethylene oxide groups. Some of the boron-based acceptors can promote the dissolution of normally insoluble salts, such as LiF, in several non-aqueous solvents. Several LiF based electrolytes of this type have been successfully evaluated in rechargeable Li/LiMnzO,, batteries.

The work on the **CRADA** with Gould Electronics, Inc. has resulted in the development of a combination of in situ high resolution XRD and XAS to study cathode materials for lithium batteries. The technique is particularly powerful for the study of transition metal oxide lithium hosts with more than one transition metal.

Impact:

This BES supported research generated two CRADAS, one with Power Conversion, Inc., the other with Gould Electronics, Inc. It also resulted in a subcontract on a Phase Il SBIR, with Technochem, Inc., on the synthesis and characterization of new lithium imide salts. These synergistic projects provide effective leverage of our BES program.

The new anion complexing agents have attracted the attention of marly organizations including IBM.

Because of our work on XAS of conducting polymers we have been asked to collaborate with PNNL on a new DOE-EM program on use of conductive polymers in nuclear waste cleanup.

Interactions:

- University collaborations include SUNY Stony Brook, Northeastern University and Polytechnic University.
- Industrial collaborations include Power Conversion, Inc., Gould Electronics, Inc., Technochem, Inc. and 3M Corp.
- Government Laboratory interactions include NRL and PNNL

Personnel:

J. McBreen (project leader), X. Q. Yang (materials characterization), H. S. Lee (materials synthesis), X. Sun (synthesis and characterization).

Recognition:

- Three invited presentations in the past year.
- Two U.S. patents awarded in past year.

Budget: $432 K