Powder Diffraction

Description: The goal of this program is to exploit high-resolution synchrotron x-ray and neutron powder diffraction techniques for structural studies of materials with interesting magnetic, electronic and catalytic properties. The characterization and development-of novel materials is critically dependent on correlating changes in their properties with changes in crystal structure as a function of temperature, pressure and composition. Frequently these effects are very subtle, involving small distortions of the lattice and small displacements of light atoms. Since suitably-sized single crystals are seldom available, the required structural information must be obtained from polycrystalline specimens in which the average crystallite size is typically about a micron. To this end, high-resolution synchrotron X-ray and neutron data are collected at state-of-the-art diffiactometers situated at beamline X7A at the NSLS and HIA at the HFBR (or at other neutron sources while the latter is shut down). The two techniques complement each other very effectively; from the synchrotron data it is often possible to detect subtle symmetry changes and solve the basic features of a previously unknown crystal structure, while the neutron data permit a precise determination of the light-atom positions, and also the arrangement of magnetic moments in a magnetically-ordered structure. Both techniques are used extensively to monitor the structural changes occurring in various types of phase transition as a function of temperature or pressure. A strong collaborative program is maintained with groups in the Department of Applied Science at BNL and with outside academic and industrial groups specializing in the synthesis of novel materials.

Program Highlights:

- Magnetic and crystallographic superstructures in La0.33Ca0.67MnO3.
- Structural changes, clustering and photo-induced phase segregation in Pr0.7Ca0.3MnO3.
- Macroscopic phase separation in Ndo.5Sro.5Mn03
- Magnetic ordering in the layered manganate Laj.4Srj.6Mn2O7
- Structure and vacancy ordering in GdBaC02051.
- Crystal structures of LaNi5-type battery electrodes.
- Charge ordering of Cu in the spin-ladder compound Srl4CU24041
- Electronic band-structure calculations and crystal structure of Sn(ND3)2F4, a precursor for NF systems.
- Electronic band-structure calculations for MNX compounds (M=Zr,Ti; X=CI,Br,l).
- Synthesis, structure and dielectric properties of Bi0.5Ag0.5Ti03-
- Predictive modeling and high-pressure high-temperature synthesis of perovskites containing Ag'+.
- Structural changes in the negative-thermal-expansion compounds ZrV207 and ZrW208.
- Fabrication of large vertically-focusing multi-wavelength neutron monochromator.

Impact:

- The work on colossal magnetoresistive manganates constitutes the most detailed and definitive crystallography of these systems to date, and has provided considerable insight into charge, orbital and magnetic ordering in La0.5Ca0.5Mn03 and La0.33Ca0.67MnO3, and the nature of photo-induced phase segregation in Pr0.7Ca0.3MnO3 and macroscopic phase separation in Nd0.5Sr0.5Mn03.
- The studies on LaNi5-type battery electrodes have contributed to the discovery of a class of Co-free and hence cheaper materials (patent pending); in addition a CRADA proposal involving similar studies aimed at improved nickel hydroxide battery electrodes has been submitted (with Energizer Power Systems).
- The development and application of synchrotron x-ray powder techniques at X7A has gained international recognition and has stimulated the construction of similar bearnlines at many other synchrotron sources.
- The neutron monochromator fabrication techniques pioneered at H I are now used worldwide.

Interactions:

- DOE laboratories: Argonne National Laboratory, Los Alamos National Laboratory.
- Universities: SUNY Stony Brook, U. of California at Santa Barbara, Oregon State U., U. of Delaware, U. of Oslo, Sendai U., Sydney U.
- Industry: Lucent Technologies, Energizer Power Systems, DuPont Corp.
- Others: ILL, Grenoble, France; MASPEC-CNR, Parma, Italy; IIS, Bangalore; RIKEN, Saitama, Japan.

Personnel: D. E. Cox (Group Leader), T. Vogt, P. Woodward (departed 9/98), E. Moshopoulou (arrived 9/98).

Recognition: (since October 1996)

* 10 invited talks at conferences, 4 seminars.
* 2 invited book chapters
* I patent pending

Budget: 305 K