
We describe powder X-ray diffraction experiments on lithium intercalation compounds of the transition metal dichalcogenides. Using a unique electrochemical cell which incorporates a beryllium window we are able to monitor changes in the host lattice which occur when the lithium concentration of the Li_xM_x2 intercalation compound is altered electrochemically. Because the X-ray diffraction experiments are performed in situ, we are also able to study dynamic processes, e.g. effects associated with the finite diffusion rate of lithium in the MX_2 host lattice. Results of experiments on Li_xTiS_2 and several other systems will be discussed. A simple theoretical model which describes the observed variation of the crystallographic c-axis with lithium content will be presented. The effect of the stored elastic energy on the electrochemical potential of the Li_xMX_2 system is calculated in mean field theory and is shown to contribute significantly to the observed variation of the electrochemical potential with lithium content.

13.X-11 X-RAY DIFFUSE SCATTERING STUDIES OF GRAPHITE INTERCALATION COMPOUNDS.* By Roy Clarke, Department of Physics, University of Michigan, Ann Arbor, MI 48109.

Graphite intercalation compounds (GIC's) display a wealth of unusual phenomena associated with the layered substructure of the intercalant. One of the most remarkable properties is the formation of long-range stacking sequences in which each intercalant layer is followed by a carbon layer to form a 'Stage n' compound. This permits the study of layers of ions in a variable environment ranging from strong 3-d coupling in the saturated materials, to a quasi 2-d situation more resembling the monolayer adsorbates, in the higher Stage compounds. A combination of photographic and diffractometer-based X-ray diffuse scattering techniques have revealed a variety of intercalant (I) substructures depending on the Stage sequence, temperature and pressure. For example, Stage 1 alkali metal GIC's display a commensurate (2x2) superlattice ordering whereas, in the higher Stages, the intercalant takes up a 2-d close-packed structure whose periodicity is unrelated to the graphite matrix. There are several interesting aspects of this structure. Most importantly, it does not have long-range intralayer order at low temperatures: instead of the usual Bragg peaks one observes a power-law X-ray profile close to a reciprocal lattice point, \( k_g \sim 1/|k-k_g|^{-2m} \) [Gavish and Imry, J. Chem. Phys. 63, 139 (1976)] reflecting an algebraic decay of positional correlations within the I-layer. The key to this behavior is interpreted to be the existence of a large density of stacking faults which induces a unique kind of disorder normal to the intercalant layers. A further unusual feature is the appearance of a phase with exponentially decaying positional correlations but with quite well-defined orientational correlations. This situation can be observed in natural single crystals of graphite intercalated with cesium and is probably an example of the 'stacked hexatic' liquid-crystal phase described by Nelson and Halperin [Phys. Rev. B 19, 2457 (1979)]. Examples of other unusual structural ordering phenomena, drawn from the acceptor-type GIC's, will be discussed. In addition to the many phase transitions that have been observed as a function of temperature, GIC's are also sensitive to changes in applied pressure and a reversible staging transition has recently been discovered using diamond-cell techniques (Clarke, Wada, and Solin, Phys. Rev. Lett. 44, 1616 (1980)).

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13.X-12 X-RAY DIFFRACTION STUDIES OF LITHIUM INTERCALATION COMPOUNDS. By B.R. Haering and J.R. Dahn, Dept. of Physics, University of British Columbia, Vancouver, B.C., Canada.

We describe powder X-ray diffraction experiments on lithium intercalation compounds of the transition metal dichalcogenides. Using a unique electrochemical cell which incorporates a beryllium window we are able to monitor changes in the host lattice which occur when the lithium concentration of the Li_xM_x2 intercalation compound is altered electrochemically. Because the X-ray diffraction experiments are performed in situ, we are also able to study dynamic processes, e.g. effects associated with the finite diffusion rate of lithium in the MX_2 host lattice. Results of experiments on Li_xTiS_2 and several other systems will be discussed. A simple theoretical model which describes the observed variation of the crystallographic c-axis with lithium content will be presented. The effect of the stored elastic energy on the electrochemical potential of the Li_xMX_2 system is calculated in mean field theory and is shown to contribute significantly to the observed variation of the electrochemical potential with lithium content.