

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 n carbon layers 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 (2×2) 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

reciprocal lattice points, \vec{k}_a , $I(\vec{k}) \sim 1/|\vec{k}-\vec{k}_a|^{2-n}$ (Gavish and Imry, J. Chem. Phys. 65, 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 R.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_xMX_2 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.

13.1-01 TIME OF FLIGHT SINGLE CRYSTAL NEUTRON DIFFRACTOMETER USING A POSITION SENSITIVE DETECTOR. By N. Niimura*, M. Arai, Y. Ishikawa, C.G. Windsor and J.M. Newsam, Laboratory of Nuclear Science*, Faculty of Science, Tohoku University, Sendai, Japan.

When the use of a linear position-sensitive detector (PSD) is combined with Time-of-Flight techniques at a pulsed neutron source, intensity data from a two-dimensional section of reciprocal space can be accumulated simultaneously. Based on this principle, we have constructed a neutron diffractometer equipped with a linear PSD proportional detector at the electron linac facility of Tohoku University. The installation of the instrument and the methods for normalising the measured intensity, decoding the position and reducing background have already been described. A research program is now underway. The spectrometer can firstly provide a qualitative picture of chosen areas of reciprocal space, allowing the observation of diffuse scattering. For example the diffuse scattering in the vicinity of (310) from a single crystal of Cu_2Mn was measured with good statistics in 6 hours enabling the short range order parameters to be deduced.

Secondly, the simultaneous measurement of data covering a range of reciprocal space allows transient or time-dependent phenomena to be examined.

Thirdly, the instrument provides a rapid means of measuring Bragg reflections, if required at several incident neutron wavelengths and over an extended range of Q . The Bragg reflections with $0\text{\AA}^{-1} < Q < 17.0\text{\AA}^{-1}$ from a single crystal of NaCl have been measured and these provide both a basis for estimating the accuracy of the method and data for the development and testing of computer programs. The present software includes routines for data correction, peak-finding and integration using data converted to reciprocal space.