PS01.06.15 ENUMERATION OF ANOMALY/PEAK BASES AND EDGE DETECTION IN TWO-DIMENSIONAL INTENSITY HISTOGRAMS. APPLICATION OF GRAPH THEORY TO CRYSTALLOGRAPHIC DATA IMAGING. Joseph H. Reibenspies, Department of Chemistry, Texas A & M University, College Station, Texas 77843 USA

Bragg peaks, spikes, intensity streaks and other anomalies generate unique domains in two-dimensional intensity histograms. Examination of the shape and edges of these domains can contribute to the identification of the type of phenomenon that generated them. The points which define the anomaly bases, when connected, with imaginary lines, will form unique base graphs. Individual base graphs, in turn, can be enumerated by employing Graph Theoretical notation and the base graph shapes classified. In edge detection, the shortest spanning tree (SST), where the tree is defined as a nonbranching, noncyclic, binary graph, can be employed. Individual domains can thus be isolated by defining their edges. Since the SST method is domain sensitive it is possible, in theory, to identify anomalies whose intensities are below the detection limit. The application of Graph Theoretical techniques to anomaly bases and edges can thus provide insight into the nature of the intensities distributed through out the two-dimensional crystallographic data image.

PS01.06.16 FEWER STRUCTURE DETERMINATION ERRORS WITH THE SMART CCD SYSTEM. Robert A. Sparks and Charles F. Campana, Siemens Energy and Automation, Inc., Analytical Instrumentation, 6300 Enterprise Lane, Madison Wisconsin 53719-1173, USA.

Data collected with the new Siemens SMART CCD diffractometer systems not only yields better quality data than conventional scintillation counter diffractometers but also leads to fewer mistakes in structure determination. The default data collection strategy used for the collection of X-ray intensity data on the SMART system involves the collection of 1.3 hemispheres of data to 0.75 resolution (at 5 cm. crystal-to-detector distance) using 10 second exposures and frame widths of 0.3 in ω. Although such a data set requires approximately six hours to complete, regardless of the size of the unit cell, the quality of data matches or exceeds that of conventional point-detector data sets collected over a much larger time periods (typically several days).

The above data collection strategy minimizes the choices which must be made by the user, thereby preventing mistakes. The determination of unit cell dimensions, reduced primitive cell, crystal system, Bravais lattice and Laue class may be done after the full data set has been collected and prior to integration. Typically, unit cell indexing is based upon 512 randomly chosen reflections and final unit cell parameters are refined from a basis set of 8192 reflections. The high sensitivity of the detector and the high degree of redundancy yields much more reliable data for evaluation of systematic absences and the determination of the correct space group. Because complete frames of data are saved, twinned and incommensurate crystals are more easily identified and in some cases structures can be determined from such crystals. Since the data set contains many redundant reflections, each with direction cosines, very good empirical or face-indexed absorption corrections may also be carried out without the need for supplemental data sets (e.g., psi scans).

Neutron Scattering I Applications

MS01.07.01 QUANTUM MAGNETIC EXCITATION IN HIGH-T_c SUPERCONDUCTORS AND THE RELATED MATERIALS. Masatoshi Arai, National Laboratory for High Energy Physics, 1-1 Oho, Tsukuba 305, Japan

Recent development of the pulsed neutron scattering technique has given very good opportunities to observe spin dynamics of low dimensional magnetic system. The magnetic dynamic structure factor in the wide range of the energy-momentum space can be observed in one time. Those were demonstrated on $KFeS_2$ [1], $KCuF_3$ [2], $CsVCl_3$ [3]. In this paper I will present on the quantum spin dynamics of the spin-Peierls system $CuGeO_3$ (T_{sp}=14K) and the high-Tc superconductor. $La_{1.85}Sr_{0.15}CuO_4$ (T_c=37K). For $CuGeO_3$ the double spin on continuum with J-10meV was clearly observed, which is surrounded by the lower boundary of the des Cloizeaux and Pearson type and the upper boundary with twice the energy and periodicity. Below T_{sp} a sharp excitation appeared at the zone boundary due to the halving of the Brillouin zone. The continuous magnetic excitation of $La_{1.85}Sr_{0.15}CuO_4$ has also observed, which extends up to 280meV. Raising temperature does not affect the dynamic property at the high energy region but at the lower energy feature around the famous incommensurate peaks. In the paper I will discuss the similarity/difference to/between the quantum excitation of the localized spin singlet pairs in the spin-Peierls state and of the itinerant RVB singlet pairs in the super conducting state.

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MS01.07.02 INELASTIC NEUTRON SCATTERING STUDIES OF DIHYDROGEN AND HYDRIDE LIGANDS IN TRANSITION METAL COMPLEXES. Juergen Eckert, MLNSC, Los Alamos National Laboratory, Los Alamos, NM 87545

Spectroscopic studies of dihydrogen and hydride ligands by inelastic neutron scattering (INS) have provided a great deal of insight in the nature of the chemical bonding of these ligands to the metal as well as important information on their local structure. In the case of the dihydrogen ligand INS can probe the hindered rotations of dihydrogen as well as metal-dihydrogen vibrational modes which have in conjunction with theoretical studies been crucial to understanding the bonding interactions of this novel ligand. This talk will cover three types of recent INS studies on hydrogen ligands: (1) the location of hydride ligands in metal clusters with large numbers of ancillary ligands by utilization of analysis of the hydride vibrational spectra; (2) information on metal-dihydrogen bonding interactions derived from extensive work on dihydrogen complexes, and the resulting implications for understanding the reaction coordinate for oxidative addition of hydrogen to the metal, and (3) some results on exchange reactions between dihydrogen and hydride ligands on the same metal.

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