

**P08.15.178***Acta Cryst.* (2008). A64, C473**Structural studies and thermal decomposition of light complex hydride**

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One of the greatest technological barriers of widespread introduction of hydrogen in global energy systems is an efficient and safe storage method. Hydrogen chemically bonded in metals or intermetallic alloys constitutes a storage alternative where very high volumetric densities can be obtained. However, in the known materials for hydrogen storage, it is always a trade-off between volumetric densities, gravimetric densities, stability, kinetics, price and safety. During the last years new hydrogen storage materials with improved properties have been synthesized and characterized. In particular novel complex hydrides based on the elements aluminium, boron, magnesium and nitrogen have been extensively studied. Alane,  $\text{AlH}_3$ , is of interest because of its very high volumetric and gravimetric hydrogen density and low decomposition temperature. 3 polymorphs (alpha prime, beta and gamma) with previously unknown crystal structures have been characterized with combined high-resolution synchrotron radiation powder diffraction (SR-PXD) and neutron powder diffraction (NPD). Their thermal decomposition behaviours were investigated by *in-situ* SR-PXD, revealing an intermingling of phase transitions and decomposition. *In-situ* SR-PXD combined with Raman spectroscopy was used to investigate thermal decomposition of  $\text{Ca}(\text{BH}_4)_2$ . The decomposition route involves several phase transitions and intermediate phases in both crystalline and amorphous state.  $\text{Li}_2\text{NH}$  is an important phase in M-Li-N-H systems but the crystal structure has been debated. NPD and SR-PXD data collected from a double isotope substituted sample,  $^7\text{LiND}_2$ , clearly show that the unit cell is larger and the symmetry is lower than the previously suggested.

Keywords: synchrotron powder diffraction, neutron powder diffraction, hydrogen storage

**P08.14.179***Acta Cryst.* (2008). A64, C473**Structures of  $\text{Li}_2\text{MnO}_3$  for lithium battery electrode materials**

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Lithium manganese oxide,  $\text{Li}_2\text{MnO}_3$ , is proposed for cathode materials of high-energy density for lithium secondary batteries.  $\text{Li}_2\text{MnO}_3$  has a rock-salt type structure with alternating Li layers and Li-Mn layers separated by closed-packed oxygen arrays. The disordered arrangements in the each layers along c-axis varied with the heat treatment temperature and the disordering affects its electrochemical property. In this study, the structure of  $\text{Li}_2\text{MnO}_3$  was studied by X-ray diffraction measurement and DIFFaX simulation for considering stacking fault in the structure. The relationship between the structures and electrochemical properties was studied. Fig. 1 shows a model of stacking fault for the Li-Mn layer used for DIFFaX simulation. The stacking of SV1 corresponds to the original

structure described by space group  $C2/m$ . In the SV2 and 2' stacking, Li exists in the Mn position by a translation of Li-Mn layer where Li and Mn exchanged. The samples heated at 600 and 800 °C were mainly composed of a random combination of SV1, 2 and 2', and the structure of the SV1', 3 and 3' was less than 10%. The electrochemical properties are discussed based on the stacking sequence.

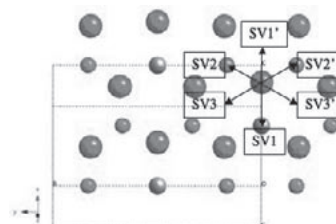


Fig.1 Stacking fault model of Li-Mn layer.

Keywords: lithium battery, stacking fault, electrode

**P08.14.180***Acta Cryst.* (2008). A64, C473**Studies of the nanostructure of natural vegetable fibers**

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Vegetable fiber is a wonder of the nature, a most important and widespread natural organic polymer. The chemical structure of the native cellulose, a basic component of the natural vegetable fiber, as a linear  $\beta$ -1,4-Glucose chain is well accepted. However, the physical structure creating the wonderful network of the supermolecular order of this fiber is not yet completely clear. From our experiments with ESR, especially with the called "ESR Spectroscopy - Tomography", in combination with other methods (X-ray diffraction, SEM, AFM, Polarized Light) on different genera of vegetable fibers (such as cotton, jute, pineapple, sisal, bamboo), we have to the first time discovered that the inside structure of the vegetable fiber is constituted not only by polysaccharide cellulose, but also by another very important component consists of fivefold [2Fe-2S] super-exchange metallo-organic combinations. These persist in the form of the composite aperiodic Nanostructures linking diagonally the cellulose chains creating an elementary fiber. A visible "macroscopic practical fiber" is constituted by a lot of the elementary fibers spiraling together about an axis by a sloping angle  $\theta = 54.7^\circ$ . This spiral angle is of a deep significance on the statistic quantum electron dynamics and the biophysical function of the fibers in the nature. This fivefold metallo-organic composite Nanostructure plays a decisive role in the specific features of vegetable fibers (such as the strength, the torsional module, the conductivity, the radiation response). On the basis of these achieved results, some physical and biological treatment techniques to improve fiber properties have been examined.

Keywords: nanostructure of natural vegetable fibers, organometallic composite nanostructure of vegetable fibers, fivefold organometallic nanostructure of vegetable fibers

**P08.10.181***Acta Cryst.* (2008). A64, C473-474**Concomitant polymorphism and twinning of dichloro-bis( $\eta$ -5-tert-butylcyclopentadienyl)titanium(IV)**

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