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Structural study of gas adsorption effects in single-walled carbon nanotubes

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Since the discovery of carbon nanotubes, it has attracted great attention to novel structural and electronic properties because of the one-dimensional structure and the tubular honeycomb network in the nanometer scale. In the viewpoint of structural properties, carbon nanotubes have inner hollow cavities with diameter typically between 1 and 20 nm, and can be filled by certain substances. This leads to interesting possible applications, such as gas absorbents and molds to form the one-dimensional (quantum) system. Especially, single-walled carbon nanotube (SWNT) are in the spotlight recently on the field of hydrogen storage due to reports of high-density hydrogen storage capability. Up to now, however, the position of stored hydrogen is still not clarified. For the gas adsorption, there are two different adosorption sites in SWNT bundle, namely the inside of SWNTs and the interstitial channels of the bundle. Here we tried to clarify the stored site of hydrogen with XRD studies at BL16XU.

The samples of SWNT bundles were synthesized by laser ablation method, and impurities were removed by H_2O_2 and HCl. Figure shows XRD patterns of *10* reflection of hexagonal lattice of SWNT bundles. Even though the clear different was not observed during storing process, the down shift of peak was detected under removing H_2 molecules from SWNTs. This phenomenon is completely opposite to that was reported in oxygen and nitrogen adsorption, where lattice expansion has been observed during adsorption. The possible mechanism for expanding lattice is still not clear and in progress.

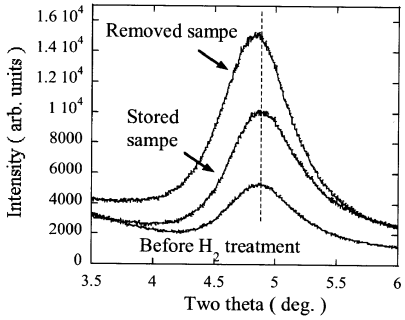

Figure. XRD patterns of *10* reflection of hexagonal lattice of SWNT bundles.

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Powder X-ray diffraction study of $LiMn_{1/2}Fe_{1/2}PO_4$

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Phospho-olivines as positive electrode materials for secondary lithium batteries are interesting materials for electrochemists and battery researchers.

Recently $LiMePO_4$ (Me=Mn or Fe) compounds have been attracting considerable attention because of its low cost and environmentally benign material compared with the first commercial material, $LiCoO_2$.

In order to use electrode materials for lithium-ion batteries, it is necessary to investigate their reaction mechanism, open circuit voltage, and thermal stability, etc. J.B.Goodenough, et al first reported Phospho-olivines as the positive electrode for secondary lithium batteries. They said that $LiMn_xFe_{1-x}PO_4$ was an excellent candidate for the cathode material.

Electrochemical properties of $LiMn_xFe_{1-x}PO_4$ depend strongly on the nature of the transition metal ion. However, it is impossible to determine the accurate position of Mn and Fe atom in olivine type structure by normal X-ray diffraction analysis. To detect the position of Mn and Fe ions in this structure, we carried out anomalous XRD by use of X-ray with different wavelength. 1.904A(6.512keV) and 1.751A(7.081keV) were chosen as energies of incident X-ray beams, which are near K edges of Mn and Fe. In this work, we try to measure $LiMn_{1/2}Fe_{1/2}PO_4$ that is typical stoichiometry in solid solutions.

$LiMn_{1/2}Fe_{1/2}PO_4$ was prepared by $LiOH.H_2O$, gamma-MnOOH, alpha-FeOOH, and $NH_4H_2PO_4$. A reaction mixture was heated at 500C in nitrogen for 6h.

Figure 1 shows the XRD patterns of $LiMn_{1/2}Fe_{1/2}PO_4$. Two diffraction patterns show the same pattern belonging to the orthorhombic cell with space group Pnma (No.62). We can not find any peak or characteristic ratio of intensity to suggest the specific positions of Mn or Fe ions in this structure.

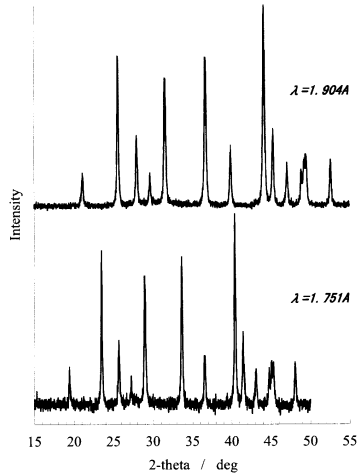

Fig.1 XRD patterns of $LiMn_{1/2}Fe_{1/2}PO_4$