EXAFS STUDY OF YMN_2D_6 SYNTHESIZED UNDER HIGH PRESSURE DEUTERIUM

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Introduction

YMn_2 compounds have been studied in detail by various groups as it possesses unusual magnetic and electrical properties. These compounds are known to crystallize in C15 cubic structure (*Fd*-3*m*) and can form hydrides or deuterides under high pressure of hydrogen or deuterium which results in transformation of structure and modification of physical properties. Synthesis of single phase YMn_2D_x (upto x = 4.5) along with structural transformation studies based on D content has been extensively studied by XRD (X-Ray diffraction), NPD (neutron powder diffraction) and EXAFS (extended X-Ray absorption fine structure) [1–3]. It is well known that magnetic properties of YMn_2 are very sensitive to Mn-Mn distances. Formation of deuteride by absorption of deuterium causes increase of cell parameters and results in structural modification which further influences magnetic properties of basic YMn_2.

We have reported the synthesis of YMn_2D_6 with high deuterium pressure and structural study has been performed both by XRD and NPD [4,5]. XRD structure refinement results show that the structure of the compound is cubic and space group is (*F*-43*m*). In which it was assumed that deuterium atoms occupying interstitial sites of AB_3, A_2B_2 and B_4 of tetrahedral structure in which experimental results show that A_2B_2 sites are most favorable sites and should be filled first before the other two sites filled up. According to NPD studies it is proved that space group of YMn_2D_6 is *Fm*-3*m* which is a super group of *F*-43*m* and better refinement results obtained.

In the present investigation we report the Mn K-edge EXAFS results of YMn_2D_6 which is necessary to get more knowledge about the short range order of atoms in YMn_2D_6. Also discussed the bond distances between Mn and Y atoms in the compound which determines the important properties.

Results and Discussion

The YMn_2D_6 sample was synthesized under high pressure of deuterium [3]. EXAFS measurement was carried out using synchrotron radiation with the electron beam energy of 1.5 GeV at the beamline of 17 C of NSRRC (National Synchrotron Radiation Research Center, Taiwan). Measurement was performed at room temperature and the photon energy was calibrated to an accuracy of 0.1 eV according to Mn metal K-edge absorption energies.

The EXAFS spectrum was refined by the program REX 2000. The atomic scattering function R(r) was calculated as the Fourier transformation of $\chi(k)$ multiplied by k^3. Single scattering r space peaks were selected, a fourier transform was calculated and least-squares fitted with an appropriate model as shown in Fig. 1.

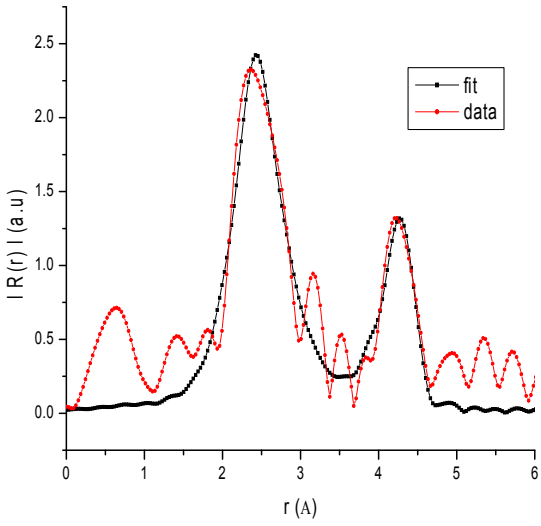

Fig 1. The EXAFS magnitudes $|R(r)|$ of atomic scattering function of YMn_2D_6 at room temperature.

The coordination numbers and interatomic distances from the core atom (Mn2) have been presented in Table 1. Interatomic distances obtained from EXAFS refinement closely resembles NPD results [5] which indicates confirmation of structural pattern positioning atoms in YMn_2D_6 based on space group *Fm*-3*m*.

Table 1. EXAFS parameters and their errors obtained from refinement

Shell	N (coordination number)	r (Å)
Mn2–Mn1	4.038 (0.03)	3.057 (0.07)
Mn2–Y	3.962 (0.03)	2.863 (0.01)
Mn2–Mn2	2.246 (0.02)	4.708 (0.04)

Figure 2 shows the schematic representation of YMn_2D_6 based *Fm*-3*m* space group which was derived from NPD data refinement [5]. Figure 1 shows two peaks for three shells which indicate the merging of Mn2-Mn1 peak and Mn2-Y peak because of reduction in bond distance of Mn-Mn and Mn-Y. Due to this shorter bond distance almost similar to $YMn_2D_{4.5}$ (around 2.9 to 3.0 Å), it is expected to have an ordered magnetic property for YMn_2D_6 also. But due to the formation octahedral cage of D atoms around Mn2 atoms prevents Mn2-Mn1 interaction and which further restricts long range ordered magnetic interactions.

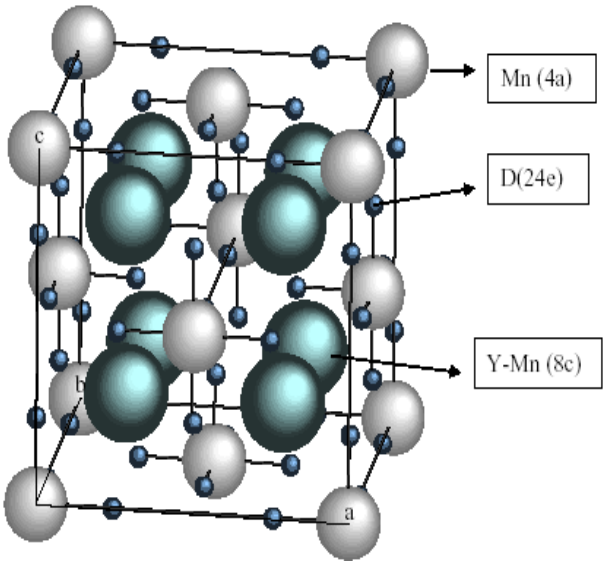

Fig 2. Crystal structure of YMn_2D_6 (*Fm*-3*m*)

Conclusions

The EXAFS measurement of YMn_2D_6 has been conducted at Mn K-edge and refinement results were analysed in continuation of our previous synthesis and characterization of YMn_2D_6 by XRD and NPD studies. It is observed that bond distances obtained by refinement results are very well comparable with NPD data.

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