Local Structure of Zirconium Complex Cross-Linked with Resin

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Zirconium salicylic acid (CAS No.226996-19-6) which is mixed with the polyester resin under heat and presser changes the physical property of the resin. It is predicted that this change is due to Zirconium atom cross-linked with resin. In this study, the Zr local structure in the polyester resin is investigated by EXAFS.

1.Experimental

The kinds of the samples of (a)～(d) are shown below.

(a) Zirconium (Ⅳ) diisopropoxidebis (2,2,6,6-tetramethyl-3,5-heptane-dionate) [obtained from Aldrich Chemical Co. Ltd. as the reference sample], (b) Zirconium salicylic acid, (c) 5% and (d) 1% Zirconium salicylic acid mixed with the polyester. Because of the low concentration of Zirconium, the sample of (c) and (d) was 1.5 and 3cm thick of the resin respectively. Zr K-Edge measurement was carried out with Si (111) double-crystal monochrometer.

2.Results

Figure1 shows the $k^3\chi(k)$ spectra and Figure2 shows the magnitude of the Fourier transform (no phase shift correction) of them. Though the transmission factor of the resin is estimated at 10% for (d), the good $k^3\chi(k)$ spectra was given to ～13 (Å^{-1}) in k-space.

Because salicylic acid has the -O-Zr-O-Zr- structure, there are two peaks assign to Zr-O (1.6Å,1st nearest neighbor) and Zr---Zr (3.1 Å ,2nd nearest) in Fig.2. The remarkably difference between (b) and (c) ～(d) is that the magnitude of the Zr---Zr for (c)～(d) is smaller than that for (b).

It is supported that the second coordination number of Zirconium atom for (c)～(d) is decreased by the reason that the Zr---Zr bonds are cut owing to cross-linking with the polyester,.

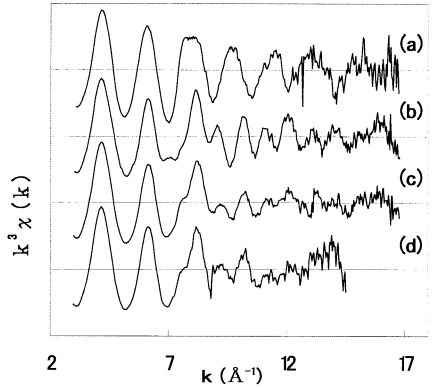

Figure 1 $k^3\chi(k)$ spectra for the sample (a)～(d)

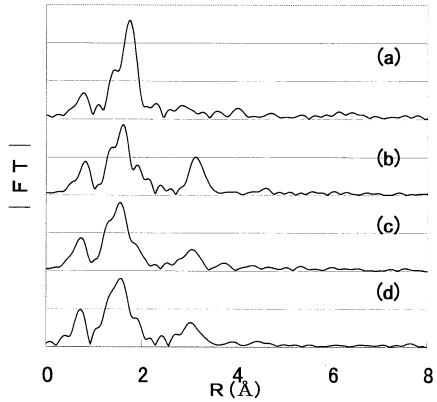

Figure 2 Fourier transforms

Change in structure of Laves phase RMn_2 compounds (R=Y,Mn) around the magnetic transition temperature

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It has been reported that the Mn atom has a large magnetic moment in the ground state in RMn_2 compounds with R=Y, Pr, Nd, Sm, Gd and Tb with relatively large Mn-Mn distance $d_{Mn\text{-}Mn}$, while it has zero or very small moment in those with R=Dy, Ho, Er, Tm and Lu with small $d_{Mn\text{-}Mn}$. Cubic Laves-phase compounds YMn_2 and $GdMn_2$ show a large spontaneous volume magnetostriction (SVM) below T_N～100K, indicating the onset of the antiferromagnetic Mn moment. In order to investigate the SVM more precisely, we have carried out the XAFS measurement on the K-edges of Y(17.0keV), Gd(50.2keV) and Mn(6.5keV) in RMn_2 (R=Y, Gd) at temperatures below 300K. The experiment was done in the transmission mode using a Si(311) or Si(111) double crystal monochromator at the BL01B1 station.

Fig. 1 and 2 show the magnitude of Fourier transform (FT) of the Y K-edge and Mn K-edge EXAFS for YMn_2 at various temperatures, respectively. Each FT spectrum is shifted properly. The correction of phase-shift is not performed. The FT up to 7 Å has clear several peaks, which are attributed to the shells shown in the figures. More detailed analysis such as a temperature dependence of the interatomic distances of Y-Y, Y-Mn and Mn-Mn is in progress.

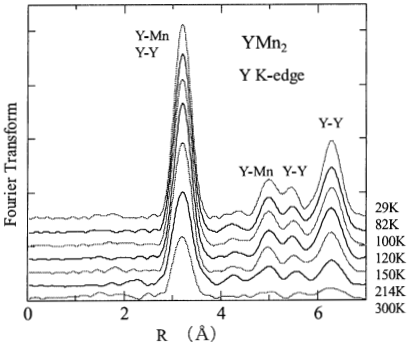

Fig.1. Fourier transforms of Y K-edge for YMn_2 at various temperatures.

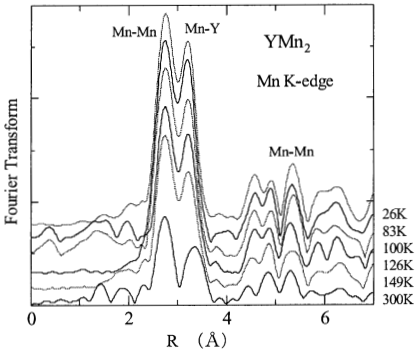

Fig.2. Fourier transforms of Mn K-edge for YMn_2 at various temperatures.