4Pa084 **Structure and Magnetic Properties of Transition Metal Acetylide Compounds MC_2 (M = Mn, Fe, Co and Ni)**

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Materials which can be used as single domain magnets attained considerable attention recently due to its application in various technological field and medicine. Apart from this, physical nature and chemistry of these materials are also scientifically interesting and important. Among these materials, transition metal carbides are potentially important for various technological applications due to its relatively low production cost as expected. However, preparation of these materials in pure form is more complicated due to the absorption of H_2O molecule. Recently Nishi *et al* developed a novel synthesis technique for the preparation of transition metal acetylede (MC_2) compounds.

The FTIR spectra of transition metal acetylyde compounds (MC_2, M = Mn, Fe, Co) are recorded using a Shimadzu, FTIR-8600PC spectrometer by KBr pellet method in the 400–4500 cm^{-1} region. The obtained spectra along with the spectrum of CaC_2 are shown Fig. 1. The IR bands corresponding to the C=C is usually observed in the region 1400 to 1500 cm^{-1} as a doublet as observed in CaC_2 (1488 and 1417 cm^{-1}). This doublet is observed in CoC_2 at 1480 and 1389 cm^{-1}. But this doublet nature is also seen in FeC_2 and appeared at 1485 and 1418 cm^{-1}. However this doublet is very small in MnC_2. Bands are observed in all the title compound in the $_2$ bending region of water at 1629, 1631 and1634 cm^{-1} in MnC_2, FeC_2 and CoC_2, respectively. The appearance C_2^{2-} bands in the IR spectra suggests the formation of transition metal acetylyde compounds. Slight changes in frequency of observed bands indicate that the bond lengths of these compounds are not uniform as expected. The presence of bending mode of water in the spectra indicates that crystalline water is adsorbed in the structure. C_{2v} molecular symmetry is suggested for MC_2 molecules by electronic structure calculations and photoelectron spectroscopy.[1] Detailed molecular symmetry of this material can be determined by doing Raman spectral measurements along with the present IR data. Transmission electron micrograph of MnC_2 is shown in Fig.2. The TEM picture shows parallel stripes in the

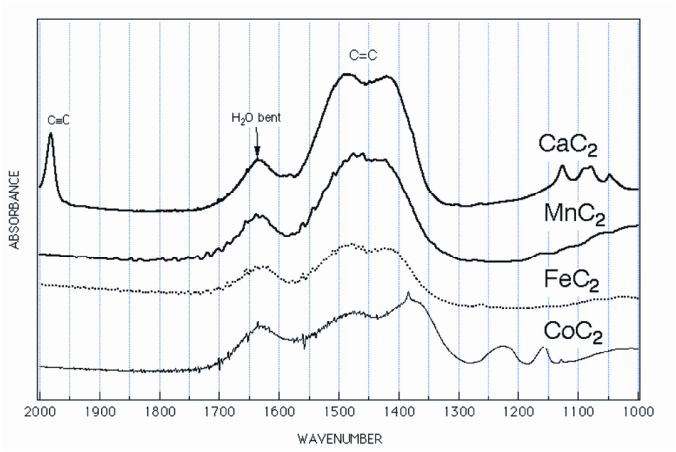


Fig. 1. FTIR spectra

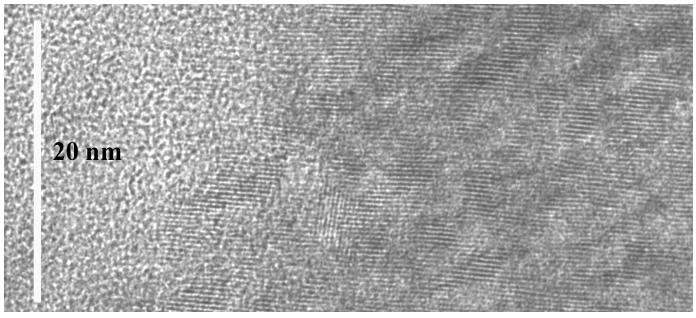


Fig. 2.TEM of MnC_2 prepared @ 190^0 C

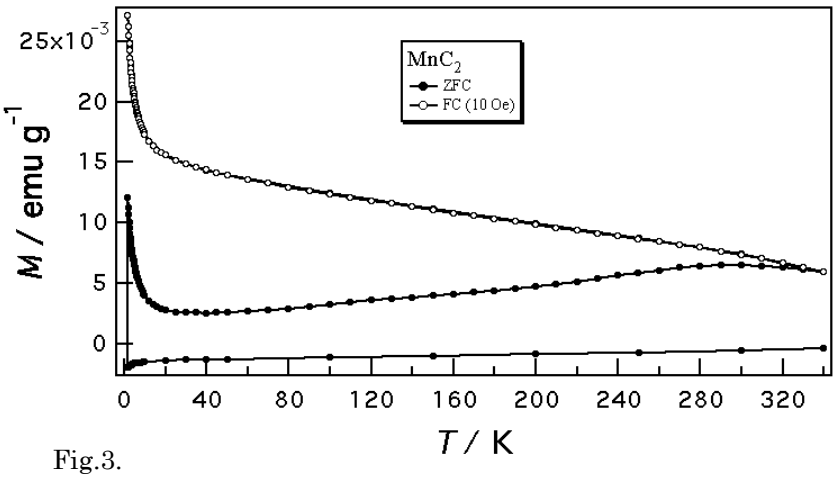
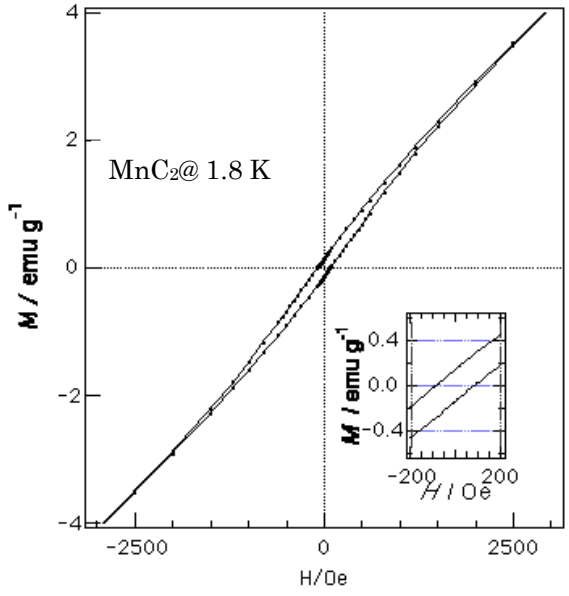


Fig.3.

material similar to NaCl structure with a step separation of 0.33 nm.

The particle size is small of the order of 2 to 3 nm. Temperature dependent magnetic measurements and hysteresis curve at 1.8 K was measured using SQUID (Quantum Design MPMS-7S) magnetometer. The observed data under zero field cooling and field cooling at 10 Oe are given in Fig.3. Under zero field cooling condition, started from 340 K, the magnetic moment is increased slightly up to 300 K, and then decreased very slowly up to 40 K and increases gradually until 12 K, then increases abruptly up to 1.8 K. But in the field cooling (10 Oe) condition, magnetic moment increases gradually up to 12 K, and then increases very rapidly until 1.8 K. The mirror image like behaviour of magnetization curve above 300 K is in agreement with cobalt carbon nanocluster magnets embedded in amorphous carbon matrix as observed by Nishi *et al.* This behaviour is due to the alignment of magnetic moments of the particles along the applied field direction. Both of the above curves meets at around 340 K suggesting a superparamagnetic to paramagnetic transition. The hysteresis curve at 1.8 K shows a coercive force of value 85 Oe that is smaller than that of CoC_2. The small crystalline domains seen in Fig.2, could be responsible for such a low value in MnC_2. The hysterysis curve at 1.8 K (Fig.4) is not saturated well showing the presence of some super paramagnetic species at this temperature also. The magnetic properties of other transition metal acetylyde compounds (MC_2, M = Mn, Fe, Co and Ni) are also studied. Preliminary studies indicate that these materials can be used for many technological applications.

Fig.4



References

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2. Nishi N, Kosugi K, Hino K, Yakoyama T, Okunishi E ; Chemical Physics Letters, **369**, 198 (2003)