



International Congress on Nanoscience and Nanotechnology  
9-11 November 2010 Shiraz - Iran

## STRUCTURE AND ELECTRICAL PROPERTIES OF $\text{CaMnO}_3$ NANOPOWDERS PREPARED BY SOL-GEL METHOD

S. Kafash, T.Ghorbani Moghadam , A.Kompany\*, S.M.Hosseini

Department of physics (Material And Electroceramics laboratory), Ferdowsi University Of Mashhad,P.O.box91775-1436,Iran

\* Corresponding Author.Tel.:+985118435723, fax:+985118796426

E-mail:ahmadkompany@yahoo.com

### KEYWORDS

Perovskite,sol-gel,calcium manganite,calcinations

### ABSTRACT

This paper describes the synthesis of  $\text{CaMnO}_3$  ceramic nanopowders by sol-gel procedure. Metal acetate precursors were used, as starting materials. Single phase perovskite structure of  $\text{CaMnO}_3$  was formed, at calcination temperature  $800^\circ\text{C}$  for two hours. The samples were characterized using XRD, UV, TEM and SEM methods. The electrical resistivity and energy band gap were also measured.

### INTRODUCTION

$\text{CaMnO}_3$  is a perovskite type oxide such and is a parent compound for many multicomponent manganites. Because of its high electrical conductivity, electrocatalytic activity and stability at high temperatures, it can be utilized as electrode materials at elevated temperatures in oxidizing atmospheres.

Also this compound has attracted attention as a possible n-type oxide thermoelectric material to be used in generators[1]. Generally ,they are interesting as electrode withdraw materials for high temperature SOFC(solid oxide fuel cell) [2]. Its crystallographic data are of importance in studies of materials having  $\text{CaMnO}_3$  as a component. Its orthorhombic structure can be treated as weakly distorted cubic one. Connected to this, the preparation of nanosized powders , that ensure a sintering at low temperature, is of great interest.

For calcium manganite the proposed conduction mechanism is a thermally activated hopping of small polarons between localized sites, $\text{Mn}^{+4}$  and  $\text{Mn}^{+3}$ . For  $\text{CaMnO}_3$ , which is a poor n-type semiconductor ,the conductivity values differ significantly in the literature,ranging from  $10^{-2}$  to  $6.3 \text{ cm}^{-1}$  at room temperature ,depending on the powder origin, sintering procedure and grain size[3],[4]. Fig. 1 shows the structure of  $\text{CaMnO}_3$  looking down the 110 axis to illustrate the out-of phase tilting of the  $\text{MnO}_6$  octahedra . The  $\text{Mn}^{+4}$  cations are at the center of the octahedral and the  $\text{Ca}^{+2}$  cations occupy the 12-coordinate sites.

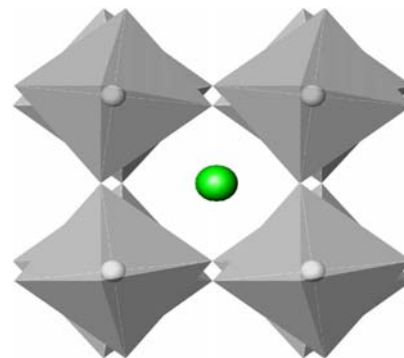


Fig.1. View of the orthorhombic perovskite structure of  $\text{CaMnO}_3$ .

### EXPERIMENTAL

Nano sized sample of  $\text{CaMnO}_3$  was prepared by sol-gel method from a stoichiometric mixture of  $\text{Ca}(\text{CH}_3\text{COO})_2 \cdot x\text{H}_2\text{O}$  and  $\text{Mn}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$  . All the synthesized powders were calcinated at  $800^\circ\text{C}$  for 2h, burning up residual organics to complete transformation into perovskite structure .  $800^\circ\text{C}$  is the lowest temperature at which perovskite structure was established. X-ray powder diffraction (XRD) analysis was carried out using  $\text{CuK}\alpha$  radiation. Scanning (SEM) and transmission electron microscopy (TEM)

techniques were used to observe the particles morphology as well as nano structures of sintered samples.

### Results and Discussion

Fig. 3 shows the resistivity-temperature characteristics of  $\text{CaMnO}_3$  nanopowders. This diagram confirms that  $\text{CaMnO}_3$  has semiconducting behavior in which the resistivity decreases with increasing temperature.

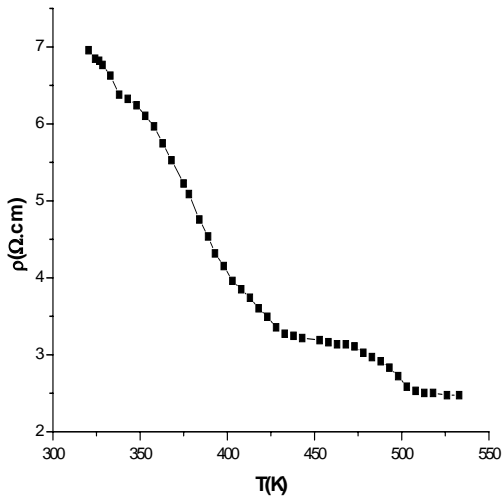


Fig.3. variation of resistivity in  $\text{CaMnO}_3$  nanopowders, as function of temperature.

In this study the UV spectroscopy was used to calculate the absorption coefficient ( $\alpha$ ) as a function of photon energy ( $h\nu$ ). The square of absorption coefficient,  $\alpha^2$ , As a function of photon energy ( $h\nu$ ) is shown in Fig.5. The value of the band gap was found to be about 3.80 eV.

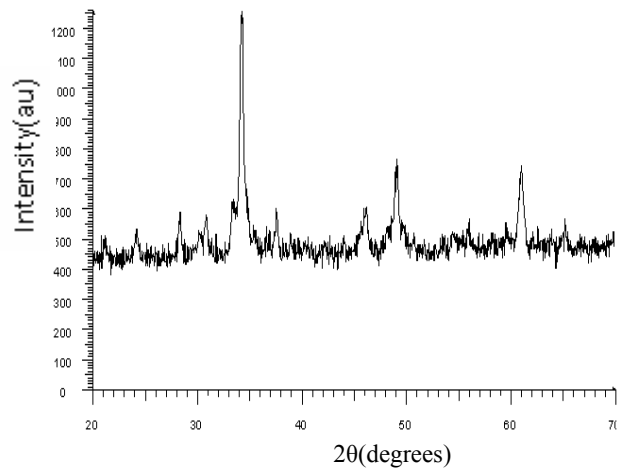


Fig.2. X-ray powder diffraction pattern of the  $\text{CaMnO}_3$  nanopowders synthesized via sol-gel technique.

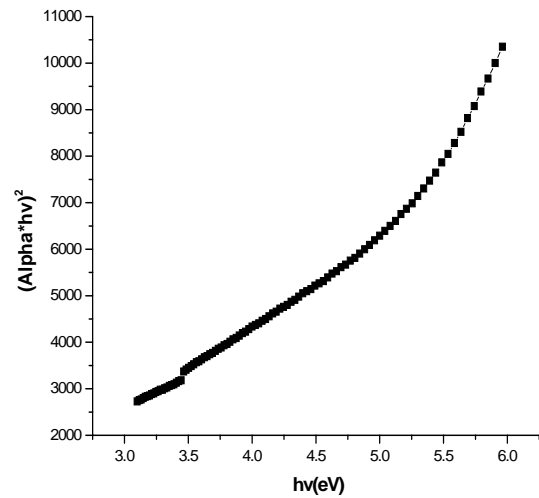


Fig.4. square of absorption coefficient, as a function of photon energy for  $\text{CaMnO}_3$  nanopowders calcinated at  $800^\circ\text{C}$ .

### REFERENCES

- [1] R. Funahashi, A. Kosuga, N. Miyasou, S. Urata, K. Lee, H. Ohta, K. Koumoto, Proc. 26th Int. Conf. Thermoelectrics, 2007, p. 124.
- [2] S.I. Vecherskii, M.A. Konopel'ko, N.O. Esina, N.N. Batalov, Transport Properties of  $\text{Ca}_{1-x}\text{MnO}_{3-\delta+x}\text{CeO}_2$  ( $0 < x < 0.15$ ) Mixtures Inorganic Materials, vol. 38, 2002, pp. 1270–1276 (No. 12).
- [3] N.N. Loshkareva, L.V. Nomerovannaya, E.V. Mostovshchikova, A.A. Makhnev, Yu.P. Sukhorukov, N.I. Solin, T.I. Arbusova, S.V. Naumov, N.V. Kostromitina, A.M. Balbashov, L.N. Rybina, Phys. Rev. B 70 (2004) 224406–224408.
- [4] C. Moure, M. Villegas, J.F. Fernandez, J. Tartaj, P. Duran, J. Mater. Sci. 34 (1999) 2565–2568.