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OPTICAL BAND GAP IN MnO-CdO-P_20_5 GLASSES

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Abstract: The phosphate glasses of composition x% MnO-[50-x]% CdO-50% P_2O_5 where $0<x<15$ and concentrations are in mole %, were prepared by melt quench technique. The optical absorption spectra for these glasses were measured in the UV-Visible spectral range. No sharp edges were found for these glasses which verifies their amorphous nature. The optical band gap energies for all these samples were calculated using the Mott and Davis relation and were found to be in the range 3.48 eV to 3.87 eV. It was also observed that the optical band gap energy decreases with increasing MnO contents.

Keywords: Mott and Davis model, optical absorbance, optical band gap energy, phosphate glasses.

INTRODUCTION

The increased demand and diverse applications of modern electronic devices have resulted in competition for cost, reliability and speed. This in turn has led to the search for new materials which can meet the specific requirements. The phosphate glasses are among these materials and have a number of technical and biological applications [Grey and Klien 1984, Kumar 1985, Nazar *et al*. 1985, Kokubo *et al*. 1986, 1991, Chen *et al*. 1993]. Such glasses containing higher concentration of rare earth ions (e.g. Mn^{+2} ions) are of special interest [Murawski *et al*. 1979] due to their potential applications in the transmission and detection of optical data. These glasses also have uses in laser technology. The electrical properties of glassy materials have been investigated and reported in literature [Ghauri *et al*. 1982]. It has been suggested that the presence of interstitials or dangling bonds give rise to a number of localized states or traps near the band edges of glassy materials. These localized states are responsible for the transport of charge carriers. At low electric fields the small polaron hopping has a dominant role [Mott and Davis 1971, Nadeem 1994] and at high field this is attributed to either Schottky (electrode-limited) [Nadeem and Hogarth 1986] or Poole-Frankle effect (bulk-limited) [Hogarth and Ghauri 1980].

The band structure of amorphous solids can be described by the C.F.O model [Cohen *et al*. 1969], which was further improved by Mott and Davis [1971]. These models provide a clear picture of the density distribution of states in the energy gap of amorphous semiconductors.

The study of optical absorption spectra provides a very useful tool for the investigation of optically induced transitions and an insight in the energy gap and band structure of crystalline and non crystalline materials. The experimental results on optical absorption in glassy materials have been reported by Mott and Davis [1971]. The optical absorption coefficient measurements have generally shown an exponential dependence on photon energy [Hogarth and Hosseini 1983]. One important difference of amorphous solids as compared with crystalline solids is that; whereas in crystalline non-metallic solids there is a sharp well defined lattice absorption edge E_g given by the relation.

$$E_g = h\,c / \lambda \qquad (1)$$

(where E_g = energy gap, h = Plank's constant, c = velocity of light), in amorphous materials the absorption edge is less sharp and is not well defined. Thus in the analysis of the variation of optical absorption with photon energy or with wave length an equation needs to be assumed to match to the experimental data. Tauc [1966] showed that the shape and position of the absorption edge for high absorption region could be represented by an equation of the form

$$\alpha(\omega) = A(\hbar\omega - E_{opt})^2 / \hbar\omega \qquad (2)$$

where α is the absorption co-efficient for non-direct transition, ω is angular frequency, A is a constant and E_{opt} is the optical energy gap.

A more general discussion of the various forms of optical absorption edge was latter given by Davis and Mott [1971], who reported a series of equations involving E_{opt}, the energy of photons involved, and the absorption co-efficient. They examined various conditions of absorption by forbidden or allowed transitions and for direct and indirect transitions in k-space. Under the assumption that k is not a good quantum number in amorphous semiconductors, they estimated the absorption co-efficient for non-direct transmission to be given by an equation of the same form as that given above by Tauc [1966]. The quadratic equation has been successfully applied by Naz [2000] to calculate the optical gap in glasses and by Nadeem and Waqas [2000] in amorphous thin layers. Here we apply the Mott and Davis theory to evaluate the optical band gap of manganese-cadmium- phosphate glass samples.

MATERIALS AND METHODS

In the present experimental work binary and ternary phosphate glasses were prepared with different compositions (Table 1). Analytical grades of CdO, MnO, P_2O_5 were used to prepare all these glasses. The appropriate amount of the constituents was calculated for 20-grams samples using the molecular weight formula of the required glass system. After weighing, the required amount of each constituent was mixed and put into the alumina crucible. The crucible was initially heated in a furnace at 500ºC for half an hour to avoid possible fuming of P_2O_5 at high temperature. It was then placed in another furnace at about 1100ºC for sample preparation and was kept at the same temperature for at least three hours. The contents were stirred with a stirrer to ensure the maximum homogeneity of the materials. Finally, the melt was quenched to form discs of different sizes. The samples were annealed at about 300ºC for three hours to eliminate the mechanical and thermal stresses.

Absorption spectra of MnO-CdO-P_2O_5 glasses with different compositions were taken using a UV-Visible Recording Spectrophotometer UV-240

Graphicord by Shimadzu, Japan. The spectrophotometer was equipped with two source beams. The frequency range covered the ultraviolet and visible radiation range.

The optical absorption coefficient $\alpha(\omega)$ was calculated for each of the specimens at various photon energies ($\hbar\,\omega$) by using the relations

$$I_t = I_o\, e^{-\alpha d} \tag{3}$$

$$\alpha(\omega) = (1/d)\ \ln(I_o/I_t) \tag{4}$$

where d is the thickness of the sample, I_o and I_t are the incident and transmitted intensities of the radiation, respectively.

Table 1: Opticla band gap energy of CdO-P2O5-MnO glasses.

Sample (Mole %)			Thickness (mm)	E_{opt} (eV)
CdO	P_2O_5	MnO		
	Binary			
50	50	00	1.63	3.87
	Ternary			
45	50	05	1.64	3.62
40	50	10	1.87	3.52
35	50	15	1.77	3.48

RESULTS AND DISCUSSION

The optical absorption spectra for CdO-P_2O_5 and MnO-CdO-P_2O_5 glasses in the UV-visible range are shown in Figs. 1-4. There is no sharp absorption edge which is a characteristic of the glassy state. The experimental value of the absorption coefficient α near the edge was calculated using Eq. (4):

$$\alpha = 2.303\ A / d \tag{5}$$

where A = normalized optical absorption and is given by $A = \log(I_o/I_t)$. The optical gap E_{opt} can be calculated from the curves representing the square root of the quantity ($\alpha\hbar\omega$) versus photon energy ($\hbar\omega$) using Eq. (1). These curves for samples having different contents of MnO and CdO are shown in Figs. 5-8. The linear part of each curve is extrapolated to the energy axis to give the value of E_{opt}. Values of E_{opt} thus evaluated are given in Table 1.

The experimental results for CdO-P_2O_5-MnO glasses show a general decrease in the optical band gap (E_{opt}) with the increasing contents of MnO. We can put the 50% CdO and 50% P_2O_5 as a reference composition. When we decrease the contents of CdO in the CdO-MnO-P_2O_5 glasses the value of optical band gap decreases. Fig. 9 gives the plot of E_{opt} versus the increasing percentage of CdO for our samples. We observe a general increase in the optical gap with increasing contents of CdO.

This may be due to certain structural changes in the material with changing composition. The increasing contents of CdO may delocalize some of the localized states present in deep energy levels [Jonscher 1967] as a result the energy gap is increased.

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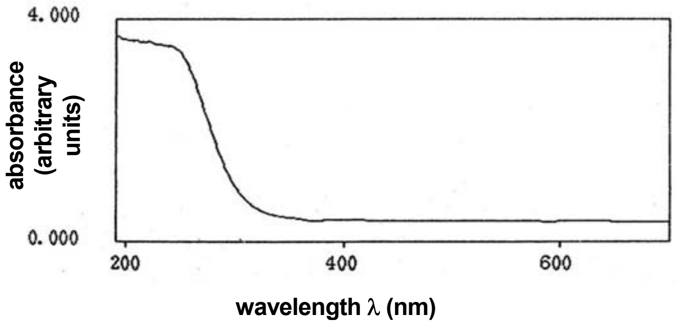

Fig. 1: Optical absorption Vs wavelength plot for 0%MnO-50%CdO-50%P_2O_5 glass.

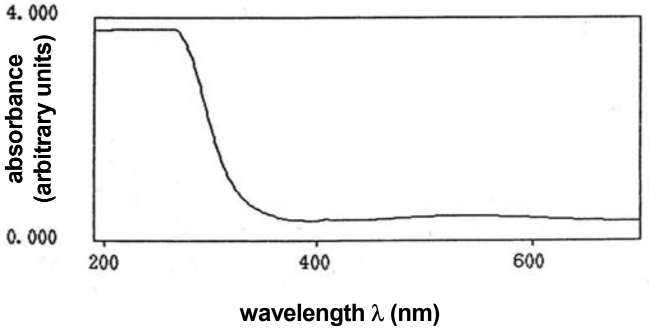

Fig. 2: Optical absorption Vs wavelength plot for 5%MnO-45%CdO-50%P_2O_5 glass.

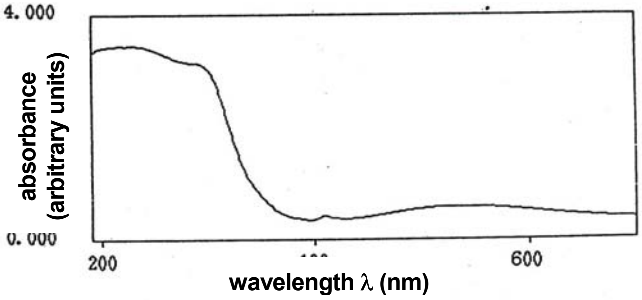

Fig. 3: Optical absorption Vs wavelength plot for 10%MnO-40%CdO-50%P_2O_5 glass.

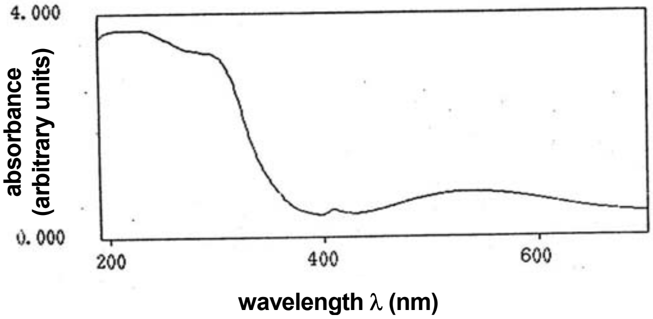

Fig. 4: Optical absorption Vs wavelength plot for 15%MnO-35%CdO-50%P_2O_5 glass.

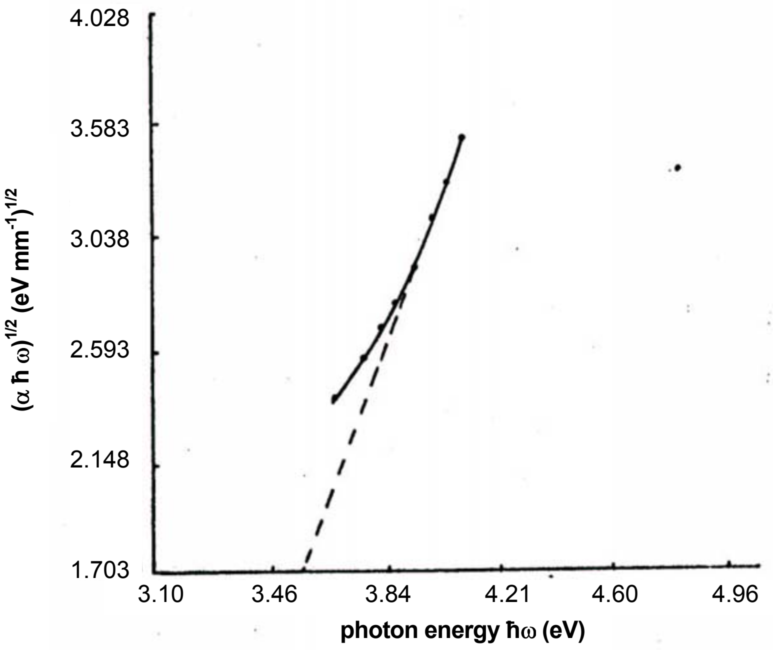

Fig. 5: Dependence of $(\alpha \hbar \omega)^{1/2}$ on photon energy for the data in Fig. 1.

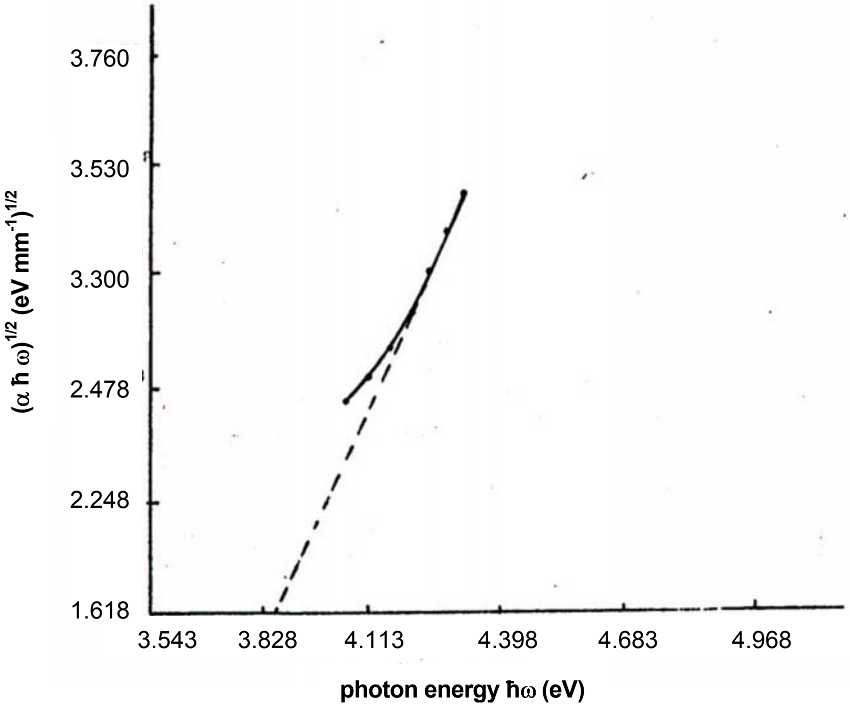

Fig. 6: Dependence of $(\alpha \hbar \omega)^{1/2}$ on photon energy for the data in Fig. 2.

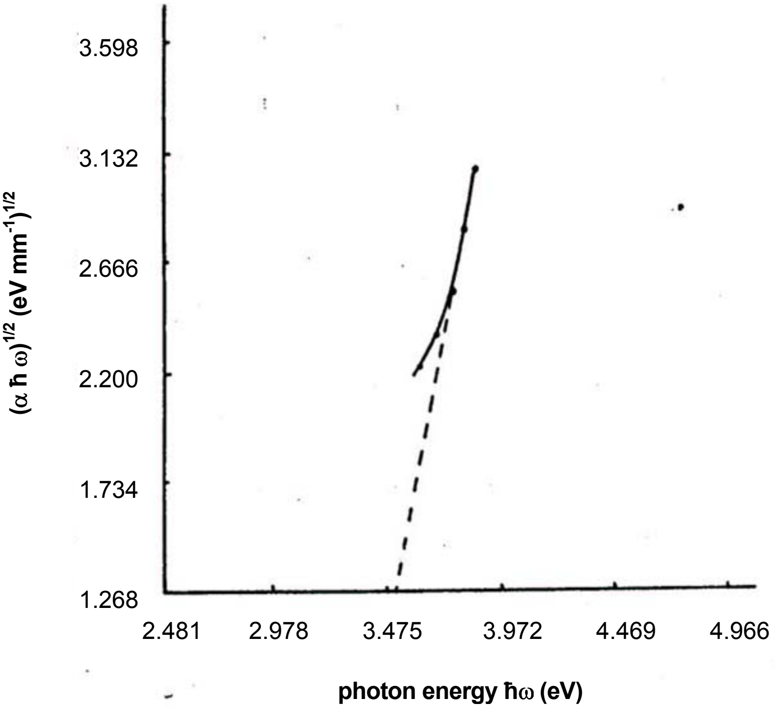

Fig. 7: Dependence of $(\alpha \hbar \omega)^{1/2}$ on photon energy for the data in Fig. 3.

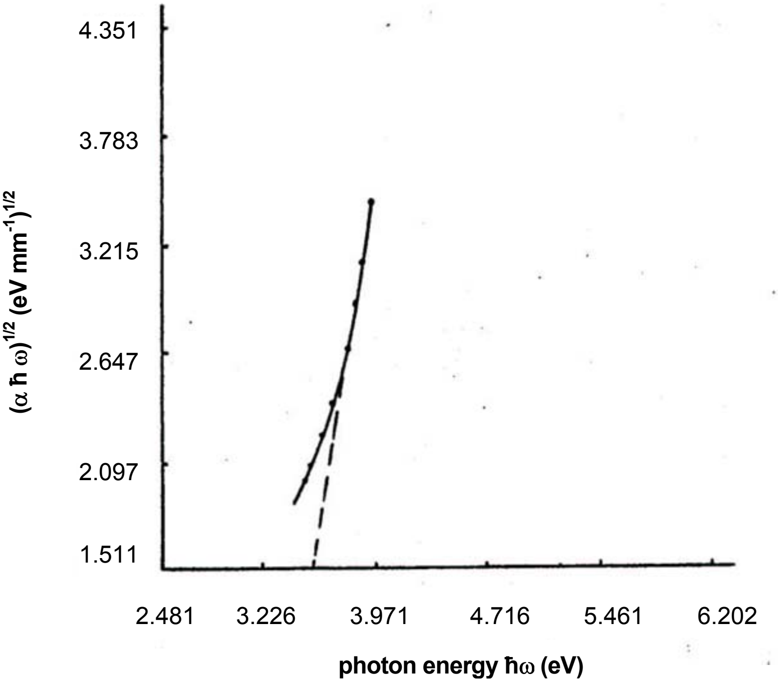

Fig. 8: Dependence of $(\alpha \hbar \omega)^{1/2}$ on photon energy for the data in Fig. 4.

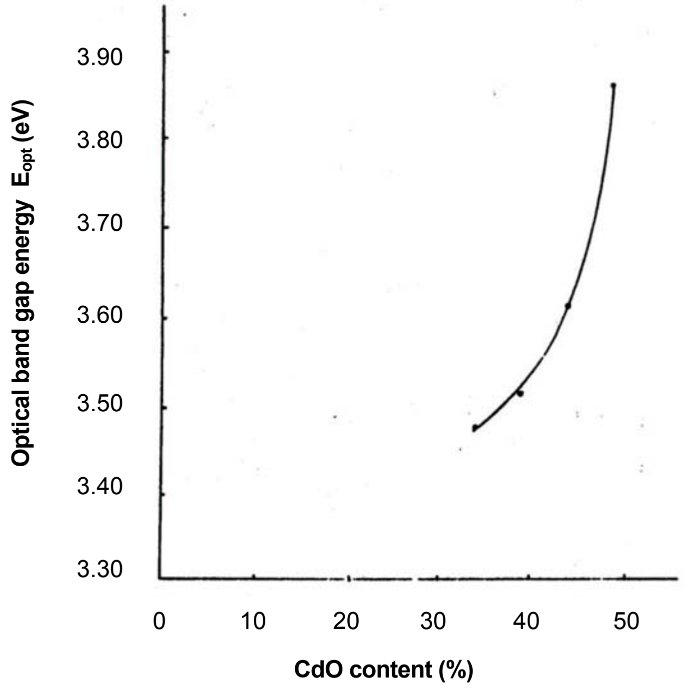

Fig. 9: Variation of the optical gap energy E_{opt} with the %age content of CdO.

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