Optical band gap of cadmium phosphate glass containing lanthanum oxide

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Summary. — Glass samples of 50% CdO-50% P_2O_5 and 5% La_2O_3-45% CdO-50% P_2O_5 were prepared by the melt quench technique. The optical absorption spectra of these samples were recorded by using Hitachi U-2000 Spectrophotometer in the wavelength 190–400 nm. The estimated value of optical band gap energy for 50% CdO-50% P_2O_5 is $\sim$ 3.45 eV and for 5% La_2O_3-45% CdO-50% P_2O_5 is 3.30 eV. The width of the band tailing, ΔE, has been estimated to be 0.26 eV and 0.47 eV for the binary and the ternary glass samples, respectively.

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1. – Introduction

Optical-absorption studies of oxide glasses provide an easy method for the investigation of optically induced electronic transitions and furnish some idea about the band structure and energy gap in such non-crystalline materials. Generally, two types [1] of optically induced transitions can occur near the fundamental absorption edge, *i.e.* direct and indirect. Both of these transitions involve the interaction between the incoming radiations and the material under investigation.

Increasing interest [2-9] exists in the study of phosphate glasses containing elements from the lanthanide series such as La, Pr, Ce, Sm etc. They find applications in electronic devices, batteries and electrochemical sensors. A literature survey would indicate that lanthanum-oxide–containing phosphate glasses have not received much attention [10], and there has not yet been published any account of the optical band gap of lanthanum phosphate binary glasses or lanthanum-containing ternary phosphate glasses.

The present work deals with the optical-absorption studies of 5% La_2O_3-45% CdO-50% P_2O_5 ternary glass and the results have been compared with 50% CdO-50% P_2O_5 binary glass sample. This study is an extension of our previous work [11-13] in which we have examined the role of ZnO on the optical characteristics of cadmium phosphate glasses.

2. – Experimental

Glass samples of 50% CdO-50% P_2O_5 and 5% La_2O_3-45% CdO-50% P_2O_5 were prepared from analytical grade CdO, $La(NO_3)_3 \cdot 5H_2O$ and P_2O_5 by the melt quench technique. The relevant amounts of glass components were taken and put into the alumina crucibles. The crucibles were initially heated in a furnace at 500 °C for half an hour to avoid the fuming of phosphorus pentoxide. The crucibles were then placed in a furnace at 1100 °C for three hours. The melts were then air quenched, in a stainless-steel die, to form disc-type samples. The samples were annealed at 300 °C to release the possible mechanical stresses produced during the casting. These samples represent their starting batch compositions in mol%. The amorphous nature of these samples has been confirmed by X-ray Diffraction Technique.

Optical absorption spectra of these samples were recorded at room temperature by using Hitachi U-2000 spectrophotometer in the wavelength range 190–400 nm.

3. – Results and discussion

The optical absorbance *vs.* wavelength curves for 50% CdO-50% P_2O_5 and 5% La_2O_3-45% CdO-50% P_2O_5 glass samples are illustrated in fig. 1. These spectra reveal that there is no sharp fall in the absorption edge with wavelength, which is an indication of the amorphous nature of the present glasses.

From the absorbance data the absorption coefficients $\alpha(\omega)$ were calculated for different photon energies by the relation $\alpha(\omega) = 2.303\, A/d$, where A is the optical absorbance and d is the thickness of the glass sample used.

The values of optical band gap energy E_{opt} can be estimated by using the equation given as

$$\alpha(\omega) = B(\hbar\omega - E_{\mathrm{opt}})^n / \hbar\omega \,, \tag{1}$$

where the exponent n has the value in the range $1/2$ to 3 depending upon the nature of interband electronic transitions. For indirect transitions $n = 2$ [1]. Values of the optical

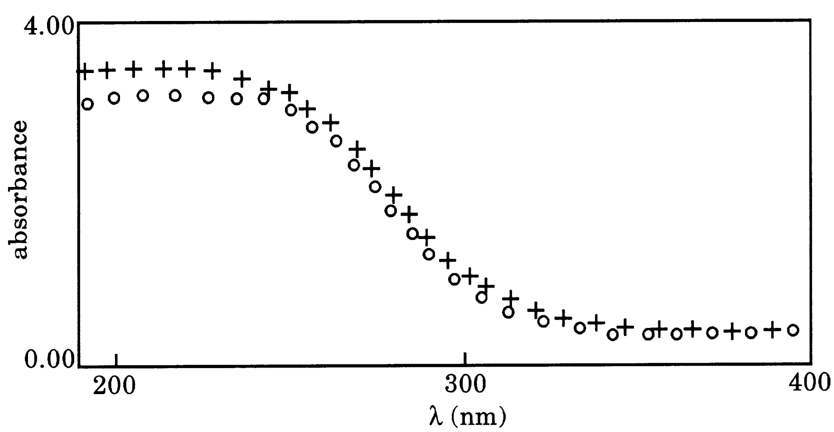

Fig. 1. – Optical absorbance *vs.* wavelength curves for 50% CdO-50% P_2O_5 glass sample and 5% La_2O_3-45% CdO-50% P_2O_5 glass sample.

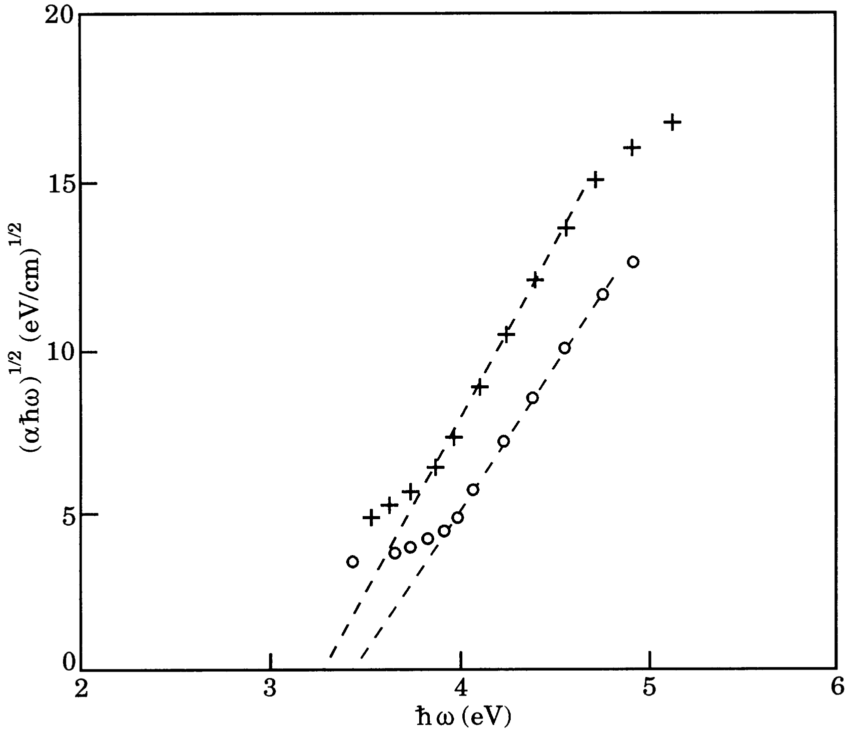

Fig. 2. – Plot of the quantity $(\alpha\hbar\omega)^{1/2}$ *vs.* photon energy $(\hbar\omega)$ for 50% CdO-50% P_2O_5 glass sample and 5% La_2O_3-45% CdO-50% P_2O_5 glass sample.

TABLE I.

Glass composition (mol %)			Thickness (mm)	E_{opt} (eV)	B $(eV \cdot cm)^{-1}$	ΔE (eV)
La_2O_3	CdO	P_2O_5				
0	50	50	2.00	3.45	69.18	0.26
5	45	50	1.43	3.30	133.95	0.47

band gaps for the glass samples were obtained by the extrapolation of linear region of the $(\alpha\hbar\omega)^{1/2}$ against photon energy $(\hbar\omega)$ plots as shown in fig. 2. This graph shows a deviation from linearity at lower photon energies which may be due to the presence of some imperfections in the material [14]. The linear relationship of $(\alpha\hbar\omega)^{1/2}$ with $\hbar\omega$ may be taken as an evidence of indirect band transition in the glasses under consideration [11]. The values of E_{opt} for binary and ternary glass samples along with the values of constant B are listed in table I. It is evident from this table that the addition of 5% La_2O_3 to the 50% CdO 50% P_2O_5 binary glass has increased the width of

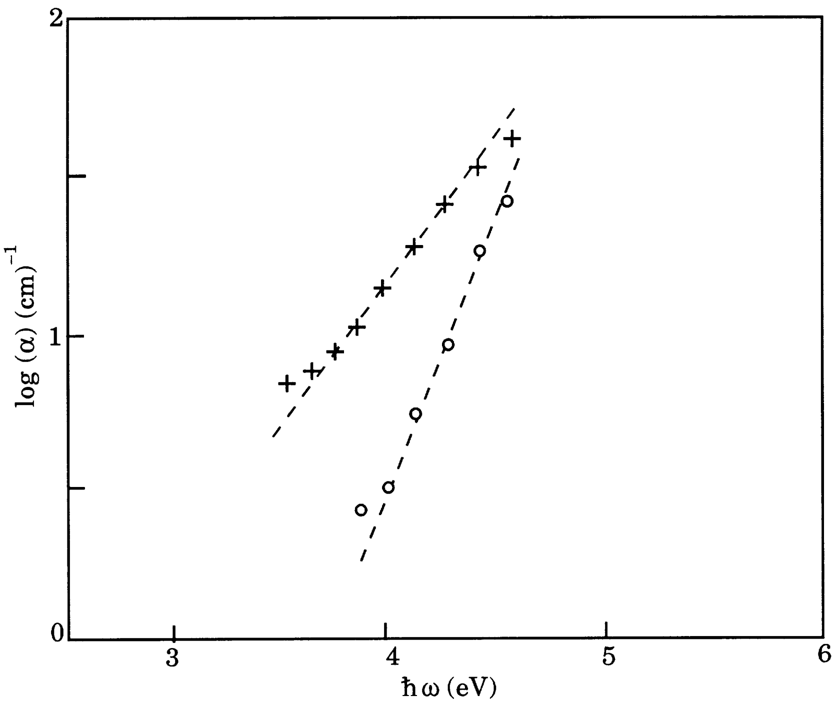

Fig. 3. – Urbach's graph for 50% CdO-50% P_2O_5 and 5% La_2O_3-45% CdO-50% P_2O_5 glass sample.

band tailing by about 0.2 eV which in turn has reduced the optical band gap roughly by the same amount, *i.e.* = 0.2 eV.

In glasses and amorphous materials there exists a band tailing in the forbidden energy band gap. The extent of band tailing is a measure of the disorder in the material and can be estimated by using the Urbach equation [15]

$$\alpha(\omega) = A \exp[\hbar\omega / \Delta E], \tag{2}$$

where A is a constant and ΔE is the width of band tails of electron states. The values of ΔE are also given in table I. The exponential behaviour corresponding to eq. (2) has also been demonstrated for the present glass samples and is shown in fig. 3.

4. – Conclusion

The following conclusions are drawn from the present work:

i) No sharp absorption edges are found for these glasses which indicate their amorphous nature.

ii) The otpical band gap of cadmium phosphate binary glass is larger than that of La_2O_3-CdOs-P_2O_5 ternary glass.

iii) The addition of 5% La_2O_3 in cadmium phosphate binary glass has *a*) decreased the band gap, and *b*) increased the width of band tails by 0.2 eV.

REFERENCES

[1] MOTT N. F. and DAVIS E. A., *Electronic Processes in Non-Crystalline Materials*, 2nd edition (Oxford Univ. Press) 1979, p. 272.
[2] MAGRUDER III R. H. and KINSER D. L., *J. Non. Cryst. Solids*, **45** (1981) 389.
[3] HARANI R., HOGARTH C. A., AHMED M. M. and MORRIS D. F. C., *J. Mat. Sci. Lett.*, **3** (1984) 843.
[4] HARANI R. and HOGARTH C. A., *J. Mat. Sci. Lett.*, **4** (1985) 399.
[5] KHAN M. N., HARANI R., AHMED M. M. and HOGARTH C. A., *J. Mat. Sci.*, **20** (1985) 2207.
[6] BRANDA F., PERNICE P., BURI A. and MAROTTA A., *J. Mat. Sci. Lett.*, **7** (1988) 218.
[7] HARANI R. and HOGARTH C. A., *J. Mat. Sci. Lett.*, 8 (1989) 150.
[8] ARZEIAN J. M. and HOGARTH C. A., *J. Mat. Sci.*, **26** (1991) 5353.
[9] COON J. and SHELBY J. E., *Phys. Chem. Glasses*, **35** (1994) 47.
[10] OHISHI Y., MITACHI S., KANAMORI T. and MANABE T., *Phys. Chem. Glasses*, **24** (1983) 135.
[11] BILAL M. S., AHMED M. A., CHAUDHRY M. A. and ALTAF M., *Mod. Phys. Lett. B*, 8 (1994) 461.
[12] CHAUDHRY M. A., BILAL M. S., ALTAF M., AHMED M. A. and RANA A. M., *J. Mat. Sci. Lett.*, **14** (1995) 975.
[13] CHAUDHRY M. A., RANA A. M., ALTAF M. and BILAL M. S., *Aust. J. Phys.*, **48** (1995) 887.
[14] REDFIELD D. and AFROMOWITZ A. M., *Appl. Phys. Lett.*, **11** (1967) 138.
[15] URBACH F., *Phys. Rev.*, **92** (1953) 1324.