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Study on Physico-Chemical Characteristics of Amorphous Structure of B_2O_3–CuO Binary System

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The B_2O_3-CuO binary system can form the glass with the percentage combinations of (100-x) B_2O_3 - (x) CuO, where x < 6. The optical edge absorption for recognizing electronic structure of this binary system has been studied. The samples were prepared from melting and then rapidly cooling of different mixtures of two oxides. The visible spectrum of these specimens in the range of 300-500 nm were characterized. The absorption coefficient $\alpha(\omega)$ is obtained by analyzing these spectra. By use of Urbach and Mott and Davis theories and tracing the diagram of $(\alpha\hbar\omega)^{1/n}$ *vs.* $\alpha(\omega)$, n = 1 was obtained. By extrapolation traced diagram of $(\alpha\hbar\omega)$ *vs.* $\hbar\omega$, the energy of optical gap, E_{opt} in $(\alpha\hbar\omega) = 0$, from 1.43 to 2.15 eV was evaluated. E_{opt} increases with increase of CuO percentages. The constant of proportion B was also evaluated by using Mott-Davis relation. The width of location state ΔE is calculated from the slop of $\ln\alpha$ *vs.* $\hbar\omega$ diagram and obtained amounts are from 0.8716 to 3.1056.

Key Words: Amorphous structures, Binary system, Optical edge absorption, Optical gap, Constant of proportion, Width of location state.

INTRODUCTION

Optical edge absorption in most of the semi-conductors have shown by $\alpha(\omega)$ which increases exponentially with $\hbar\omega$. The variations of absorption coefficient with energy of photon in high energies, takes an exponential tail[1]. Edge absorptions of amorphous layers has a slope less than the crystalline forms.

In most of amorphous substances the edge absorption classified in two categories:

(1) High absorption zone [$\alpha(\omega) > 10^4$ cm^{-1}]; the absorption coefficient calculates by following equation:

$$\alpha(\omega) = B\frac{\left(\hbar\omega - E_{opt}\right)^n}{\hbar\omega} \quad (1)$$

where B is constant of proportion, E_{opt} is energy of optical gap, ω is angular frequency of transmitted ray and n is 1, 2 or 3/2 which depends to type of electronic transition in K space. This equation is proposed by Tauc *et al.*[2] with n = 2 and then by Mott and Davis[3] with n = 3/2.

(2) Low absorption zone [$\alpha(\omega) < 10^4$ cm^{-1}]; the absorption coefficient varies exponentially with energy of descent photon ($\hbar\omega$). The most convenient equation which describes optical behaviours of amorphous substances was proposed by Urbach[4],

$$\alpha(\omega) = C \exp \frac{(\hbar\omega)}{\Delta E} \quad (2)$$

where C is proportion constant and ΔE is width of location state in bonds of energy.

EXPERIMENTAL

Method of preparation the samples: The samples of B_2O_3-CuO binary system were prepared by melting well mixed of B_2O_3 and CuO oxides mixtures as defined in Table-1.

TABLE-1
PERCENTAGES OF EACH COMPONENT IN PREPARED SAMPLES

Sample no.	B_2O_3 wt. %	CuO wt. %
1	98.5	1.5
2	97.5	2.5
3	96.5	3.5
4	95.0	5.0

As increase in percentage of CuO, softening point increases, thus a specimen with 3 wt. % CuO fluidized at 700 ºC, but one with 7 wt. % CuO fluidized at 750 ºC.

Visible spectra of these samples show that they are vitreous structure, because the spectrum of an amorphous solid has not sharp edge absorption (Fig. 1).

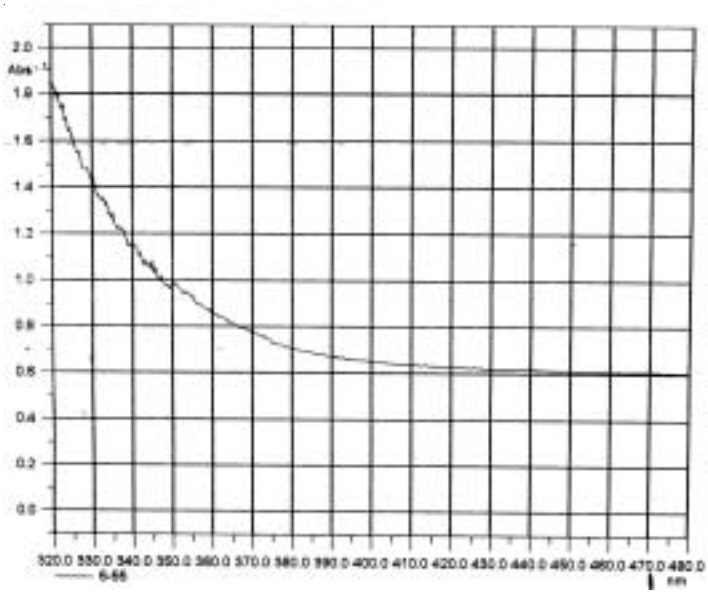

Fig. 1. Visible spectrum of sample No. 3, 3.5 wt. % CuO, thickness 0.96 mm

RESULTS AND DISCUSSION

For calculating absorption coefficient $\alpha(\hbar)$ we have traced these diagrams and then taken 10 points over the visible spectrum of each sample and obtained $\alpha(\omega)$ by use of following equation[5],

$$\alpha(\omega) = \frac{1}{L} \times 2.303 \log \frac{I_0}{I} \tag{3}$$

where L is the thickness of sample, I_0 and I are the energies of descent and absorbed photon, respectively. Angular frequency ω evaluated by use of following relation,

$$\omega = 2\pi - \frac{c}{\lambda} \tag{4}$$

where c is the velocity of light in vacuum.

The $\alpha\hbar\omega$ and $\hbar\omega$ values were calculated and then plotted the diagram of variation $(\alpha\hbar\omega)^{1/n}$ *vs.* energy of descent photon $\hbar\omega$, for different amounts of n (n = 1, 2 and 3/2). The diagrams show that the diagram for n = 1 have better exponential tail than the others. By extrapolating this diagram, the optical gap energy E_{opt}, at $\alpha\hbar\omega = 0$ was determined. The slope of the diagram gives the constant of Mott-Davis relation B (Fig. 2).

The diagram of ln α(ω) *vs.* $\hbar\omega$ was plotted. Inverse of the slope of this diagram gives the width of location state (Fig. 3).

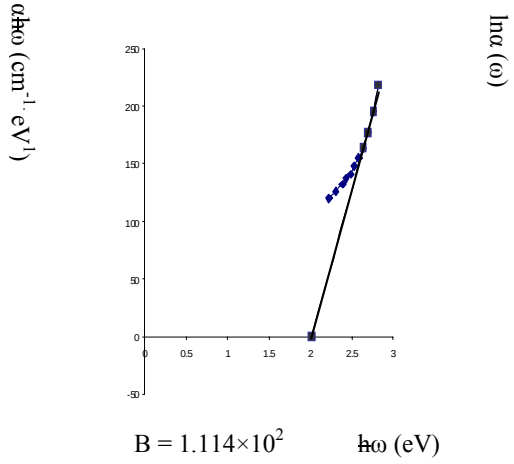

Fig. 2. Diagram of variation of α ω *vs.* $\hbar\omega$ for sample no. 3, 3.5 wt. % CuO thickness 0.96 mm

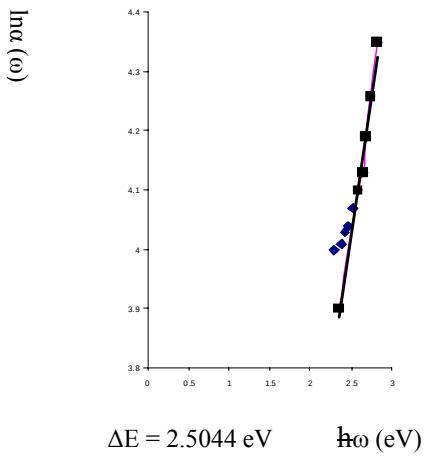

Fig. 3. Diagram of variation of ln α(ω) *vs.* $\hbar\omega$ for sample no. 3 3.5 wt. % CuO

Experimental results and evaluations for all of samples are shown in Table-2.

TABLE-2
EXPERIMENTAL RESULTS AND EVALUATIONS FOR ALL OF SAMPLES

Sample no.	Wt. of oxides		Thickness (mm)	E_{opt} (eV)	B (cm^{-1} ev^{-1} × 10^2)	ΔE (eV)	Type of transition
	B_2O_3	CuO					
1	98.5	1.5	0.61	1.43	0.740	3.1056	Not allowed
2	97.5	2.5	0.64	2.01	1.526	1.7634	Not allowed
3	96.5	3.5	0.96	1.79	1.114	2.5044	Not allowed
4	95.0	5.0	0.82	2.15	1.971	0.8716	Not allowed

Conclusion

Study on spectra of samples favour with vitreous structure, because there is no sharpness in their edge absorption. The given experimental data showed that the edge-absorption tend to short views-high energies-when CuO percentage increase, which shows increasing of optical gap energy. This is probably due to Cu^{+}/Cu^{2+} ratio. Same results have obtained for V_2O_5-CeO_2 binary system and Randall and Rooksly[6] related this effect to V^{4+}/V^{5+} ratio.

Increasing the thickness of each sample with the same percentage of CuO, causes increase of width of location state ΔE and decrease of optical gap energy E_{opt}. Studying MoO_2-In_2O_3 binary system, Anwar and Hosseini[7] obtained analogue results with the results of Ashrafi *et al.*[8]. This effect is related to the fact that increasing the thickness of a sample increase overlap of electronic wave functions. Consequently, there is increasing of width of location state and it follows that, increasing of optical gap energy.

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