Electrical and optical properties of $\text{MoO}_3\text{--V}_2\text{O}_5$ mixed oxide films

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Abstract. Vacuum deposited $\text{MoO}_3\text{--V}_2\text{O}_5$ films of different molar concentrations have been used for DC electrical conductivity studies at different temperatures. The optical absorption spectra of $\text{MoO}_3\text{--V}_2\text{O}_5$ films of different molar concentrations have been measured. From these measurements it is found that optical band gap and activation energy vary with molar concentration of $\text{MoO}_3\text{--V}_2\text{O}_5$ films.

Keywords. $\text{MoO}_3\text{--V}_2\text{O}_5$; activation energy; mixed oxides; optical band gap.

1. Introduction

The dielectric films are important for manufacturing semiconductor devices and integrated circuits. Charge transport measurements in semiconductors and insulators have been of considerable interest recently, because they can provide information about electronic structure of amorphous materials. The study of mixed thin films of $\text{MoO}_3\text{--V}_2\text{O}_5$ has been made and reported here.

Anwar and Hogarth (1990) studied various properties of mixed oxide systems of $\text{MoO}_3\text{--In}_2\text{O}_3$ and $\text{MoO}_3\text{--SiO}_2$ thin films. Chopra *et al* (1990) reported electrical and optical properties of amorphous films of $\text{V}_2\text{O}_5\text{--TeO}_2$ systems by varying molar percentage composition of each oxide. Khan and Hogarth (1990) investigated electrical and optical properties of $\text{V}_2\text{O}_5\text{--B}_2\text{O}_3$ mixed oxide amorphous thin films. Kang *et al* (1989) studied mixed oxide system of $\text{V}_2\text{O}_5\text{--MoO}_3$. Several authors (Najbar and Nizioi 1978; Eon *et al* 1979) have reported the type of reaction of $\text{V}_2\text{O}_5\text{--MoO}_3$ to be as follows:

i.e. (i) During absorption of atomic oxygen the V_2O_5 and V_2MoO_8 phases coexist; and (ii) under desorption of oxygen the $(\text{Mo}_{0.3}\text{V}_{0.7})_2\text{O}_5$ phase is formed.

These are the reversible solid state reactions in the case of $\text{MoO}_3\text{--V}_2\text{O}_5$ mixed oxide system.

The optical properties of evaporated thin films of $\text{MoO}_3\text{--V}_2\text{O}_5$ system has been studied. The optical absorption is a useful method for the investigation of optically induced transition and the provision of information about the band structure. The principle of this technique is that photons with energy greater than the band gap energy will be absorbed. The optical energy gaps of a number of mixed oxide films have been successfully analyzed on the basis of the theory proposed by Davis and Mott (1970) and Tauc *et al* (1966) for amorphous materials.

2. Experimental

Analytical reagent grade MoO_3 and V_2O_5 powder of various molar concentrations have been taken in an agate mortar and ground well to get a fine powder of the mixed oxide, which is then pelletized. These pellets have been used for EBG evaporation in a vacuum unit at a pressure of 8×10^{-4} Pa onto cleaned glass and mylar substrates. The substrates have been kept at a temperature of 100°C . Thickness of the film has been monitored on a thickness monitor and accurately measured by Tolansky's method. Films of 90% MoO_3 :10% V_2O_5 , 75% MoO_3 :25% V_2O_5 , 60% MoO_3 :40% V_2O_5 and 50% MoO_3 :50% V_2O_5 have been used for optical and electrical investigations. In the case of optical studies UV-visible spectra (Shimadzu 160A Spectrophotometer) have been taken. For electrical studies coplanar electrical conductivity variation of these films have been made using the Keithley Electrometer (Model No: 617).

3. Results and discussion

The electrical studies have been made for the films of different percentage of molar concentrations. Assuming an Arrhenius type relationship,

$$\sigma = \sigma_0 \exp(-\Delta E/k_B T), \quad (3)$$

Figure 1. Plot of $\ln \sigma$ vs $10^3/T$ for MoO_3 - V_2O_5 system in different molar concentrations. Thickness of the films is in between 190–210 nm.

Table 1. Activation energy of mixed systems of MoO_3 and V_2O_5 of various molar concentrations.

Sample	90% MoO_3 : 10% V_2O_5	75% MoO_3 : 25% V_2O_5	60% MoO_3 : 40% V_2O_5	50% MoO_3 : 50% V_2O_5
Activation energy (eV)	0.716	0.338	0.263	0.029

Figure 2. Transmittance spectra of $\text{MoO}_3\text{-V}_2\text{O}_5$ system in different molar concentrations as a function of wavelength. Thickness of the film is in between 190–210 nm.

where σ_0 is the pre-exponential factor and k_B the Boltzmann's constant, ΔE the thermal activation energy. Figure 1 gives the plot of $\ln \sigma$ vs $10^3/T$ of 90% MoO_3 :10% V_2O_5 , 75% MoO_3 :25% V_2O_5 , 60% MoO_3 :40% V_2O_5 and 50% MoO_3 :50% V_2O_5 films of almost the same thickness (190–210 nm). The increase in conductivity and decrease in activation energy, when the molar percentage of V_2O_5 increases in MoO_3 , is attributed to the increasing concentration of oxygen vacancies and vanadium interstitials. The value of activation energy in the lower temperature region is due to the electronic hopping process which dominates lower temperature conduction in the samples. The straight line part of the curve in the high temperature region corresponds to activation energy. The conduction in high temperature is believed to be a transition from hopping conduction to a free band conduction. The gradual transition from hopping to free band conduction may be due to overlapping of localized levels and free bands.

In amorphous materials both free band and hopping conduction may take place as in crystalline materials (Anwar and Hogarth 1990). These conduction mechanisms may be separated experimentally by operating in the appropriate temperature ranges.

As the value of V_2O_5 is increased in MoO_3 its activation energy decreased, which is shown in table 1. In other words, when the content of V_2O_5 is increased, the conductivity increases. Thus, when the content of V_2O_5 increases the concentration of trapping centres of MoO_3 decreases and the conductivity of the mixed film increases.

The transmittance spectra for $\text{MoO}_3\text{-V}_2\text{O}_5$ system taken using UV-visible spectrophotometer are shown in figure 2. Data from figure 2 are used for plotting $(\alpha\hbar\omega)^{1/n}$ vs

Figure 3. Plot of $(\alpha\hbar\omega)^{1/2}$ vs $(\hbar\omega)$ for different molar concentrations of MoO_3 and V_2O_5 mixed system. The thickness of the film is 190–210 nm.

Table 2. The optical band gap of mixed oxide systems of MoO_3 and V_2O_5 in various molar concentrations.

Sample	90% MoO_3 : 10% V_2O_5	75% MoO_3 : 25% V_2O_5	60% MoO_3 : 40% V_2O_5	50% MoO_3 : 50% V_2O_5
Optical band gap (eV)	2.856	2.748	2.354	2.123

$\hbar\omega$ in accordance with equation (Tauc *et al* 1966; Tauc 1972),

$$(\alpha\hbar\omega) = B(\hbar\omega - E_{\text{opt}})^n, \quad (4)$$

where n is an exponent, ω the angular frequency of the incident radiation, h the Planck's constant, B a constant and E_{opt} the optical energy gap of the material. The exponent n can take the values 2, 3, $1/2$, and $3/2$ for indirect allowed, indirect forbidden, direct allowed and direct forbidden transitions respectively. Plotting $(\alpha\hbar\omega)^{1/n}$ vs $\hbar\omega$ and extrapolating to $(\alpha\hbar\omega)^{1/n} = 0$ yields the value of E_{opt} which is in reasonable agreement with the available values of Donnadiou *et al* (1988) (2.80 eV) and, Khan and Hogarth (1991) (2.10 eV) for MoO_3 and V_2O_5 respectively.

Here $n = 2$ gives maximum points on the best fit line as shown in figure 3. The optical band gaps have been evaluated (table 2). When the molar percentage of V_2O_5 is

increased in the mixed oxide system there is an overall disorder in the system. Vanadium ions may be incorporated in an MoO₃ lattice. The presence of interstitial vanadium ions in the MoO₃ lattice may cause a decrease in the optical band gap. This result supports the idea that in MoO₃–V₂O₅ films, indirect transitions occur with stronger absorption because the *k* vector is not uniquely defined in disordered materials.

4. Conclusion

From the present work the optical transmission minima of amorphous MoO₃–V₂O₅ film are observed to be governed by direct forbidden transition. The optical band gap and activation energy decreases with incoming molar concentration of V₂O₅ in the system.

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