Optical absorption in co-evaporated V$_2$O$_5$–TeO$_2$ thin films

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The electron diffraction pattern shows that co-evaporated V$_2$O$_5$–TeO$_2$ thin film samples are amorphous at room temperature and become polycrystalline at temperatures higher than about 513 K. This behaviour is similar to that of amorphous V$_2$O$_5$ thin films. The optical absorption edge of amorphous thin films of V$_2$O$_5$–TeO$_2$ is studied in the wavelength range 200 to 900 nm and the FTIR spectra are studied in the wave number range 400 to 4000 cm$^{-1}$. The FTIR spectra of amorphous V$_2$O$_5$ thin film are found to be similar to those of amorphous V$_2$O$_5$–TeO$_2$ thin films. This suggests that the coordination number of the vanadium ion in V$_2$O$_5$–TeO$_2$ is the same as that in crystalline V$_2$O$_5$, and thus the optical absorption edge of amorphous V$_2$O$_5$–TeO$_2$ thin films can be described by direct forbidden transitions.

1. Introduction
In all band models of amorphous semiconductors, the localized states due to the lack of the long-range order, are close to the band edges rather than deep in the bands. Most of the workers [1, 2] agreed that the states are localized below $E_c$ and above $E_v$ which are sharply defined energies called the mobility edges [1]. These localized states play an important role in determining the optical absorption edge and their contribution to the optical transitions may be seen through the following arguments. Davis and Mott [3] derived an equation for the optical absorption coefficient $\alpha(\omega)$ as a function of photon energy $h\omega$

$$\alpha(\omega)h\omega = B(h\omega - E_{opt})^n$$

where $n$ is an exponent, $\omega$ the angular frequency of the incident radiation, $B$ a constant and $E_{opt}$ is defined as the optical energy gap of the material and corresponds to the smallest energy separating the localized states that are close to one of the two bands and the extended states of the other (see the model of Davis and Mott [3]).

A similar equation with $n = 2$ was derived by Tauc et al. [4]. The definition given to $E_{opt}$ by these authors is, however, different from that given by Davis and Mott. Tauc et al. defined it as the energy separating the localized states above $E_c$ and those below $E_v$.

Equation 1 with $n = 2$ offers the best fit to the optical absorption data in most amorphous semiconductors. There are, however, special cases where the index $n$ is different from 2. For instance Davis and Mott [3] gave the value $n = 1$ in amorphous selenium and many other workers found $n = 3/2$ in vanadate glasses. It is thought that this value is due to the fact that the coordination environment of V$^{4+}$ in crystalline V$_2$O$_5$ is not affected by the disorder. Indeed nuclear magnetic resonance studies show that the coordination number of the vanadium ions in the glass is the same as for the vanadium ions in crystalline V$_2$O$_5$ [5, 6] and that their site symmetry is similar to that in the crystal. As a consequence, one would expect similar electronic transitions in both non-crystalline and crystalline V$_2$O$_5$. In fact, it was found in the latter (V$_2$O$_5$ single crystal) that the absorption coefficient fits the condition for direct forbidden transitions

$$\alpha h\omega = B(h\omega - E_{opt})^{3/2}$$

much better than it fits the condition for direct allowed transitions [7, 8] given by

$$\alpha = B(h\omega - E_{opt})^{1/2}$$

Al-Ani and Hogarth [9] have also used Equation 2 to determine the optical gap of V$_2$O$_5$–SiO$_2$ amorphous thin films and they found that it gives a better fit to their optical absorption data. In addition the optical absorption properties of V$_2$O$_5$–P$_2$O$_5$ glasses show that the fundamental absorption arises from direct forbidden transitions (Equation 2) and occurs at about 2.4 eV at room temperature [10].

Equations 2 and 3, give very different plots for the optical absorption data. The choice between equations 1 (with $n = 2$) and 2 becomes difficult in the case where both of them give straight lines. The aim of this paper, therefore, is to compare Equations 1 (with $n = 2$) and 2 with the help of the FTIR studies, so that we can choose the appropriate equation for the calculation of the optical energy gap.

2. Experimental work
The optical absorption measurements of co-evaporated V$_2$O$_5$–TeO$_2$ thin films in vacuum of 10$^{-6}$ torr, were made in two spectral regions; the ultraviolet and the infrared region (4000 to 400 cm$^{-1}$). Corning 7059 glass substrates were used for the UV, and monocrystalline silicon wafers were used as substrates for the FTIR measurements. The optical measurements in
the ultraviolet and visible regions were made using a Perkin-Elmer (Model Lambda 3) double beam spectrophotometer and the infrared measurements were made using a Perkin-Elmer (Model 1710 FTIR) double beam spectrophotometer. The effects of the substrate on the UV and FTIR characteristics were minimized by placing another cleaned uncoated substrate in the path of the reference beam. The structure of layers of about 40 nm thickness was investigated in an electron microscope (JEO model JEM7) by electron diffraction and microscopy. For this purpose the thin film of $\text{V}_2\text{O}_5$–$\text{TeO}_2$ was deposited on a carbon-coated mica substrate held at room temperature.

3. Results and discussion
Curves of the optical transmittance as a function of wavelength for different compositions of $\text{V}_2\text{O}_5$–$\text{TeO}_2$ co-evaporated layers are presented in Fig. 1. It is seen that the transmittance is very low indicating

Figure 1 Optical transmittance as function of wavelength for $\text{V}_2\text{O}_5$–$\text{TeO}_2$ thin films (about 200 nm thick). (a) 68%$\text{V}_2\text{O}_5$ and (b) 51%$\text{V}_2\text{O}_5$.

Figure 2 (a) $(\sigma\omega)^{1/2}$ and (b) $(\sigma\omega)^{2/3}$ plotted against $\omega$ for $\text{V}_2\text{O}_5$–$\text{TeO}_2$ thin films (about 200 nm thick). (a) 68% $\text{V}_2\text{O}_5$ and (b) 51% $\text{V}_2\text{O}_5$.

Figure 3 FTIR absorbance plotted against wave number for (a) $\text{V}_2\text{O}_5$–$\text{TeO}_2$, (b) $\text{V}_2\text{O}_5$ and (c) $\text{TeO}_2$ thin films.