



International Journal of ChemTech Research CODEN (USA): IJCRGG ISSN : 0974-4290 Vol.6, No.7, pp 3931-3934, Sept-Oct 2014

# Thermal Evaporated V<sub>2</sub>O<sub>5</sub> Thin Films: Thermodynamic Properties

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**Abstract:**  $V_2O_5$  has been intensively investigated as a cathode material for rechargeable lithium-ion batteries because of its low cost, abundance, easy synthesis and high energy density. It is a typical intercalation compound with a layered crystal structure with a large variety of atomic and molecular species that can be reversibly intercalated and extracted between the layers. Many methods of preparation, physical and chemical methods are used to prepare  $V_2O_5$  thin films: chemical vapor deposition, magnetron sputtering, sol-gel technology, thermal evaporation technique and flash evaporation. Hence in the present study, thin films of  $V_2O_5$  were prepared by thermal evaporation and the structure and thermo emf of the prepared samples were studied. The diffraction pattern of  $V_2O_5$  thin films deposited at room temperature indicating that the structure is amorphous in nature. The plot of thermo emf versus temperature difference between the two junctions is found to be linear indicating that the temperature dependence of thermo emf is the characteristic conduction of the films.

Keywords: V<sub>2</sub>O<sub>5</sub> thin films, Thermal, Structure and Thermo emf.

# Introduction:

Thin films of semi-conducting materials generally have neither the same physical properties nor the same chemistry as the respective bulk material. Moreover, the preparing techniques and deposition processes used to create films dramatically change the physical properties of material such as refractive index, extinction coefficient, homogeneity, density, hardness, internal stress, adhesion to substrate and crystal structure. Therefore, the difference in physical properties between bulk and thin film material depends strongly on many factors such as the type of deposition process itself, deposition temperature, deposition rate, gas pressure, substrate geometry and preparation of the coating material and the post-deposition temperature [1]. Transition metal oxides have been a subject of research in recent years in view of their fundamental and technological aspects. Among these, vanadium creates many compounds with oxygen; these have different structural, optical and chemical properties. Meaningful differences between the properties of different phases of vanadium oxides like VO,  $VO_2$ ,  $V_2O_3$  and  $V_2O_5$  depend on their structure, which determines other properties. Different forms of vanadium oxides can be obtained by changing the deposition process parameters, or by post-process treatment, e.g., additional annealing. From the application point of view, the most interesting vanadium oxides are VO<sub>2</sub> and  $V_2O_5$ . Vanadium dioxide is a very good candidate for thermochromic coatings due to the change of properties from semiconducting to semimetal at 68°C. Vanadium pentoxide ( $V_2O_5$ ) is a thermodynamically stable form which exhibits electrochromic properties.  $V_2O_5$  thin films can also be used in optical filters,

reflectance mirrors, smart windows and surfaces with tunable emittance for temperature control of space

In the past decade, nanostructured vanadium oxide compounds have attracted much interest due to their chemical and physical properties and their great potential for applications in catalysis [2] as sensors [3] in electro chromic devices [4] in electrochemistry [5] in photo catalytic activities [6] and in spintronic devices [7]. Among the various vanadium oxide compositions that can be obtained,  $V_2O_5$  possesses a unique set of properties and is one of the most widely studied of the more stable phases of vanadium oxides [8]. Because its structure is composed of two-dimensional layers, this material is also used as an intercalation compound. Since the reversible electrochemical lithium ion intercalation in  $V_2O_5$  was first reported in 1976 [9] vanadium pentoxide has been intensively investigated as a cathode material for rechargeable lithium-ion batteries because of its low cost, abundance, easy synthesis, and high energy density. It is a typical intercalation compound with a layered crystal structure, with a large variety of atomic and molecular species that can be reversibly intercalated and extracted between the layers. However, the development of rechargeable lithium-ion batteries with vanadium pentoxide as a cathode has been limited for its poor structural stability, low electronic conductivity and ionic conductivity and slow electrochemical kinetics.

When  $V_2O_5$  intercalates  $Li^+$ , electrical energy stores in the electrode. Energy releases from the electrode when Li+ diffuses out. For electrochemical pseudo capacitor applications, the charge/discharge rate and the energy storage capacity are the most important parameters. Larger surface area and easy charge transport are required to achieve high charge/discharge rate [10, 11]  $V_2O_5$  xerogel and aerogel, both offer large surface area, have been explored for such application and have demonstrated a current density of 6 C (C is about 150 mA h/g  $V_2O_5$ ) without storage loss. However,  $V_2O_5$  xerogel and aerogels are well-known to suffer from their structural stability; the porous structure readily collapses during  $Li^+$  intercalation and extraction processes. Thermal evaporation is one of the most widely used, simplest and convenient techniques for the deposition of thin films. In this technique, the material can be evaporated by means of resistive heating or rf heating. This is done in a high vacuum, both to allow the vapour to reach the substrate without reacting with or scattering against other gas-phase atoms in the chamber, and to reduce the incorporation of impurities from the residual gas in the vacuum chamber. Hence in the present study  $V_2O_5$  thin films were deposited by thermal evaporation method and the structure, thermo emf of the samples were studied.

## **Experimental:**

vehicles.

 $V_2O_5$  thin films were prepared on to Corning 7059 glass substrates by thermal evaporation of pure  $V_2O_5$ Powder (purity 99.99% obtained from MERCK) from an electrical heated molybdenum boat kept at ~ 1823 K in a vacuum better than 8 x 10<sup>-6</sup> Torr. A Hind High Vacuum 12A4 Coating unit was used for the deposition of the experimental films. A diffusion pump backed by a rotary pump was employed to produce the ultimate pressure of 3 x 10<sup>-6</sup> Torr. Well cleaned Corning 7059 glass substrate along with suitable masks were mounted on a copper holder which was fixed on a tripod in the beljar. The source to substrate distance was fixed at 15 cm. After getting the ultimate vacuum of 5 x 10<sup>-6</sup> Torr and the desired substrate temperature in the chamber, the glow discharge was initiated further ionically clean the substrates in the vacuum chamber. This was done for about two minutes. The system was allowed to reach the ultimate vacuum. When the power was fed to the boat, the material in the boat evaporated and the vapours reacted with the oxygen gas leading to film deposition on the substrate. The temperature of the boat during deposition was monitored by means of an optical pyrometer [12].

The substrates were maintained at the required deposition temperature and then, the molybdenum boat in which  $V_2O_5$  powder was kept. The shutter covering the substrates was opened when the temperature of the boat reached about 1823 K and it was maintained during the deposition of the films. The deposition rate observed by a quartz crystal thickness monitor was 10 A<sup>0</sup>/sec. The structure of  $V_2O_5$  thin films was analyzed using a Philips X-ray diffractometer with CuK $\alpha$  ( $\lambda = 1.5418$  A<sup>0</sup>) target. The X-ray diffraction profiles were recorded in the scanning angle range 10-80<sup>0</sup> with a scanning speed of 1 deg./ min. The thermo emf of the prepared samples was studied between the temperature ranges from 275 to 325 K by using thermal probe method.

#### **Results and Discussion:**

The deposition parameters such as substrate temperature, deposition rate, film substrate combination, vacuum during the film deposition etc. greatly influence the physical and chemical properties of the oxide thin

films. In the present investigation thin films of  $V_2O_5$  were prepared on Corning7059 glass substrates keeping all the deposition parameters fixed except the substrate temperature.

**Structure:** The X-ray diffraction profiles were recorded in the scanning angle range  $10-80^{\circ}$  with a scanning speed of 1 deg./min. The X-ray diffraction pattern of room temperature deposited V<sub>2</sub>O<sub>5</sub> films assured their amorphous nature. Fig. 1 shows a typical XRD pattern of one of the as deposited V<sub>2</sub>O<sub>5</sub> thin films.



Fig. 1 XRD pattern of  $V_2O_5$  thin films deposited at room temperature

**Thermo emf:** The thermo power or Seebeck coefficient, of a material measures the magnitude of an induced thermoelectric voltage in response to a temperature difference across that material and the entropy per charge carrier in the material [13]. The term "thermo power" is a misnomer since it does not measure power, but measures the voltage induced in response to a temperature difference. An applied temperature difference causes charged carriers in the material to diffuse from the hot side to the cold side. Mobile charged carriers migrating to the cold side leave behind their oppositely charged nuclei at the hot side thus giving rise to a thermoelectric voltage. The material's temperature and crystal structure influence S; typically metals have small thermo powers because of half-filled bands caused by equal negative and positive charges cancelling each other's contribution to the induced thermoelectric voltage. In contrast, semiconductors can be doped with excess electrons or electron holes, causing the magnitude of S to be large. The sign of the thermo power determines which charged carriers dominate the electric transport. The temperature difference  $\Delta T$  between the two ends of a material is small and then the thermo power of a material is defined approximately as:

$$S = -\Delta V / \Delta T$$

and a thermoelectric voltage of  $\Delta V$  is seen at the terminals.

The thermo emf of laser deposited  $V_2O_5$  thin film was studied in the temperature range from 275 K - 325 K by using thermal probe method is given in Table-1.

 Table-1
 Thermo emf versus temperature

Temperature (K)	Thermo emf (µV)
	0.045
275	0.265
280	0.547
285	0.738
290	0.925
295	0.989
300	1.154
305	1.478
310	1.687
315	2.287
320	2.922
325	3.435

The thermo emf was measured and the Seebeck coefficient of the material was also calculated. The plot of thermo emf versus temperature difference between the two junctions is found to be linear (Fig.2) indicating that the temperature dependence of thermo emf is the characteristic conduction of  $V_2O_5$  films. The thermo emf of  $V_2O_5$  films increased with the increasing of temperature. At low temperatures the Seebeck coefficient is observed to be high and the Seebeck coefficient decreases with increasing of temperature. The large values of thermoelectric power of  $V_2O_5$  thin films are typical of semiconductor behavior.



Fig. 2 Temperature dependence of the thermo emf of  $V_2O_5$  thin film

## **Conclusions:**

Thin films of  $V_2O_5$  were prepared by thermal evaporation method. The strucure and thermo emf of the prepared samples were studied. The diffraction pattern of  $V_2O_5$  thin films deposited at room temperature indicating that the structure is amorphous in nature. The plot of thermo emf versus temperature difference between the two junctions is found to be linear indicating that the temperature dependence of thermo emf is the characteristic conduction of the films.

#### Acknowledgements:

The author (M. C. Rao) is thankful to UGC for providing the financial assistance through Major Research Project (Link No. F. No. 40-24/2011(SR)).

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