Thermophysical Properties of Silver Doped V₂O₅ Thin Films

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Abstract—In this work we investigate structural, electrical and thermoelectrical properties 0, 1 and 3% Ag doped V_2O_5 thin films fabricated by inorganic sol gel method on quartz substrates. XRD analysis demonstrates that the films are polycrystalline and comprised of orthorhombic V_2O_5 phase. Grain size calculated from the full width at half maxima of these peaks shows that crystallite size decrease with Ag doping. Resistance vs temperature shows that all the samples exhibit semiconducting behaviour and resistance decrease with Ag doping. Hall measurement demonstrates that carrier concentration increases with increase in Ag doping where as mobility decreases. Thermoelectrical studies show that magnitude of Seebeck coefficient increases with increase in Ag doping percentage. Variation of transport studies have been understood by Trapping and filtering of charge carriers by grain boundaries.

Keywords: *V*₂*O*₅, *Seebeck coefficient*.

1. INTRODUCTION

Vanadium oxides offer many convenient physical effects which can be used for different microelectronic device applications [1]. Vanadium is a multivalent element and as a result forms variety of oxides upon reacting with oxygen such as VO, V_2O_3 , VO_2 , V_6O_{11} , V_2O_5 etc. V_2O_5 is the saturated (highest oxidation state) in the V-O system and consequently the most stable one among these vanadium oxides [2-3]. It has a lamellar, or sheet like structure. It is a distorted orthorhombic structure, and this deformation creates its sheet formation. V_2O_5 in the form of thin films has attracted much attention due to its unique electronic, chemical and optical properties. Metal to insulator transition (MIT) at approximately 280 °C in V2O5 by lattice distortion and a structural inhomogeneity due to the vanadyl-oxygen vacancies reported recently [4–6], makes V₂O₅ a promising material for thermoelectric devices. V₂O₅ exhibits highly anisotropic electrical and optical properties due to its orthorhombic structure and these properties have been extensively investigated by many researchers. On the other hand, the thermophysical properties including thermal conductivity (κ), Seebeck coefficient (s), and dynamic heat capacity have received less attention. In the present paper we present thermophysical properties of Ag doped V_2O_5 thin films.

2. EXPERIMENTS

Thin films of V_2O_5 on quartz substrates were fabricated by simple and cost effective inorganic sol gel method. Complete details of fabrication of thin films is discussed somewhere else [7]. X-ray diffraction (XRD) measurements at room temperature in the 20 range 20–60^o is carried out to identify the crystalline phases and structure of the films using a Bruker D8 advance diffractometer with Cu Ka (0.15406 nm) X-ray source at a scan speed of 0.5° min⁻¹. The electrical resistance (R) and Seebeck coefficient (*S*) of these films are measured in the temperature range 300–400 K using a standard DC four probe and bridge method respectively. The Hall effect measurements are carried out in the same temperature range by Ecopia HMS-3000 Hall Measurement System to evaluate charge carrier density (*n*) and mobility (μ).

3. RESULTS AND DISCUSSIONS

1. X-ray Diffraction

Figure 6.2 (a-d) shows the XRD patterns of Ag doped V_2O_5 thin films. Diffraction patterns of undoped thin film can be indexed to polycrystalline orthorhombic V_2O_5 phases [JCPDS file no. 85-0601].



Figure 1: XRD pattern of samples.

No significant change appears in the crystal structure due to incorporation of Ag ions in the crystal lattice of V_2O_5 . The relative high intensity of the (001) peak demonstrates the growth of films are oriented along the c-axis perpendicular to the surface of substrate. In addition to (001) Braggs reflection, the subsequent appearance of other characteristic orientations such as (101), (110) and (002) reveal the existence of in-plane orientation of V-O-V chains. Table 1 presents the crystallite size (D) calculated by well know Scherrer formula and interplanar spacing (d) of thin films. It is evident from the table that D decreases whereas d increases with increase Ag doping. Increase in d is due to replacement of V ions by Ag ions in V₂O₅ since the radius of V is smaller than the Ag. No peak corresponding to Silver or silver oxide was observed which is due to the fact that the Ag atoms in doped samples play the role of the solute donor forms a solid solution phase in the V_2O_5 thin film.

TABLE 1: Various calculated parameters of samples.

Sample	D(nm)	d (Å)
Undoped	27.4	4.31
1% Ag doped	22.6	4.34
3% Ag doped	14.5	4.36

2. Electrical Transport Studies

Temperature dependence of resistivity (ρ) of thin films in the temperature range 300-400 K is shown in Figure 2. All the samples show semiconducting behavior as electrical resistivity decrease with increasing temperature. Doping of Ag in the V₂O₅ lattice reduces the resistivity.



Figure 2: Resistivity as a function of Temperature.

Figure 3 shows variation of n and μ . Carrier concentration increases with Ag doping, whereas carrier mobility decreases with Ag doping.



Figure 3: *n* and μ of samples

Figure 4 displays the variation of *S* as a function of temperature for Ag doped V_2O_5 thin films. Negative value of *S* shows that all the samples posses N-type conduction mechanism. With increase in temperature magnitude of *S* increases. In the entire temperature range magnitude of *S* increases with Ag doping.



Figure 4: S as a function of Temperature

Increase in electrical conductivity with Ag doping can be understood as. Ag acts as a charge donor impurity in the V_2O_5 lattice thus increases the *n* and hence the electrical conductivity of V_2O_5 thin films. Variation of μ and *S* can be explained on the basis of trapping and scattering of charge carriers along the grain boundaries. As discussed in the XRD spectra that crystallite size decrease with Ag doping and this increases the size of grain boundaries. These grain boundaries acts as potential barrier and traps out the low energy charge carriers as shown in fig 5. The magnitude of S value depends on the mean carrier energy relative to the Fermi level [8]. Therefore, this phenomenon of filtering of charge carriers also leads to an increase in S. Scattering of charge carriers by grain boundaries results decrease in μ with Ag.

4. CONCLUSIONS

From last few years researchers are trying to search out thermoelectrical materials of metal oxides as conventional thermoelectrical materials are unstable at higher temperatures. Thermoelectrical performance of material is measured by Power factor given by $P = S^2 \sigma$. Practically V_2O_5 posses good value of *S*, but small value of σ makes V_2O_5 in convenient to use for thermoelectrical applications. Doping of silver into V_2O_5 thin films simultaneously increases *S* and σ and thus enhances thermoelectrical performance of V_2O_5 thin films.



Figure 5: Schematic Diagram showing filtering of charge carriers along grain boundaries.

5. ACKNOWLEDGEMENTS

One of the authors (BA) would like to acknowledge MHRD for providing the research fellowship and IUAC, New Delhi for samples preparation and their characterization.

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