Optical and electrical investigations of a-GaTe nanoparticles thin films prepared by inert gas condensation technique

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Amorphous gallium telluride nanoparticles thin films have been deposited on glass substrate using inert-gas condensation technique. Structural characteristics have been carried out by X-ray diffraction, scanning electron microscopy and field emission transmission electron microscopy. These observations show that the prepared samples are amorphous, possess aggregates and have particle size in the range of 20–75 nm. Optical band gap and Urbach energy of samples were determined using UV-visible absorption spectroscopy. The optical absorption edge was described through electronic transition model proposed by Tauc. The bandgap is allowed direct type and is ~ 2.29 eV. DC electrical conductivity of thin films was measured in temperature range of 345-525 K and the activation energy for dc conduction process was estimated. The obtained data indicated that prepared samples behave as semiconductor material and the electrical conduction is through a thermally activated process.

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1. Introduction

Nanoscience and nanotechnology involve studying and working with matter on a nanoscale. The study of nanoparticle systems has been a subject of continuous interest in Physics as well as in other disciplines [1-3]. The essence of nanotechnology is the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new properties. It is concerned with materials and systems whose structures and components exhibit novel and significantly modified physical, chemical, and biological properties, phenomena, and processes due to their nanoscale size. Such new forms of materials and systems/devices herald a revolutionary age for science and technology, provided we can discover and fully utilize the underlying principles [4].

The amorphous nano-particles/structures may yield a greater variety of properties than that of crystalline nanoparticles/structures because the bonding constraint arising from crystalline unit cells does not exist in them. Hence, chalcogenides glasses appear to be interesting materials for investigations at nanoscale. Chalcogenide glasses have gained much importance because of the presence of electronic conduction that makes them suitable for electronic devices. Recently, several workers [5-13] reported the synthesis of semiconductor nanoparticles/structures using different methods and their characterization. However, studies on nano-chalcogenides are still at the beginning, and accordingly, overall features have not been discovered. Understanding the optical and electrical processes in chalcogenide compounds such as

GaTe at nanoscale is of fundamental importance both from scientific and technological point of view.

To the best of our knowledge, the application of inert gas vapor condensation technique for the preparation of amorphous gallium telluride ultrafine powder has not been previously described. Moreover, a-GaTe thin films has been deposited using inert gas condensation (IGC) method; and characterized with X-ray diffraction (XRD), scanning electron microscopy (SEM), field emission transmission electron microscopy (FETEM), UV-visible absorption spectroscopy and electrical transport measurements. The present study concentrates on the structural, optical and electrical properties of amorphous gallium telluride nanoparticles thin films.

2. Experimental details

The unit used for the synthesis of a-GaTe ultrafine powder consists of high vacuum chamber pumped to a residual vacuum of ~ 10^{-6} torr. Pellets of commercially available GaTe (Sigma Aldrich, 5N purity) were evaporated on cooled copper substrates using tantalum boat. Argon gas was used at pressure of 0.5 torr. The material was collected on a liquid nitrogen cooled copper substrate and passivated with oxygen before opening the chamber to air. Furthermore, good quality thin films (thickness ~ 600 nm) of amorphous gallium telluride nanoparticles have been deposited by vacuum evaporation technique onto ultrasonically cleaned glass substrates in a vacuum of ~ 10^{-6} torr. The previously evaporated material was deposited on a glass substrate which was pasted on liquid nitrogen cooled copper platform. Such ambient conditions make the nature of samples amorphous. Thickness of the films has been measured using a quartz crystal thickness monitor.

The prepared films were checked using X-ray diffractometer (Phillips X'Pert) with CuK_{α} radiation $(\lambda = 1.54056\text{\AA})$. Morphological and microstructural studies were carried out with SEM images, obtained with SEM (JEOL SM-6340 F) and TEM images, obtained with FETEM (JEOL JEM-2100F). Optical absorption spectra obtained using UV-visible double were beam spectrophotometer (Hitachi, U-3501) in wavelength range 200-1100 nm. For dc conductivity measurements, two thick indium electrodes were deposited on the film by vacuum evaporation technique. The samples were then mounted in a specially designed metallic sample holder where a vacuum of about 10^{-3} torr could be maintained throughout the measurements. A dc voltage (1.5 V) was applied across the sample and the resulting current was measured by a digital electrometer (Keithley, 617).

3. Results and discussion

3.1 Structural studies

X-ray diffraction pattern of a-GaTe nanoparticles thin film is shown in the inset of Fig. 1(a). No significant peak has been observed in XRD pattern which exhibits the amorphous nature of the sample. SEM micrograph of a-GaTe nanoparticles thin film showing its surface morphology is presented in Fig. 1(a). From SEM micrograph, it is observed that the film possesses aggregates of nanoparticles and some pinholes. FETEM image showing the microstructure of a-GaTe nanoparticles is presented in Fig. 1(b). It is clear from this image that all the particles are distinguishable, almost spherical and their size varies from 20-75 nm.



Fig. 1. (a) SEM micrograph of a -GaTe nanoparticles thin film and inset shows XRD of the same. (b) FETEM image of a-GaTe nanoparticles thin film.

3.2 Optical studies

UV-visible absorption spectra of a-GaTe nanoparticles thin film are shown in Fig. 2. The absorption coefficient (α) of the film, which is displayed in inset of Fig. 2, was determined from absorbance data using the relation:

$$\alpha = \frac{A}{d} \tag{1}$$

where A is absorbance and d is thickness of film. In amorphous semiconductors, optical absorption spectra have been found to have three distinct regions viz a high absorption region, an exponential edge region, and a weak absorption tail region.



Fig. 2. (a) Absorbance spectra of a-GaTe nanoparticles thin film and (b) inset shows Absorption coefficient vs. photon energy for the same.

In high absorption region (where $\alpha > 10^4$ cm⁻¹), which involves electronic transitions between valence and conduction bands, absorption coefficient is described according to electronic transitions model proposed by Tauc [14], by the relation:

$$\alpha h \nu = B(h\nu - E_g)^P \qquad (2)$$

where hv, E_g and B are the photon energy, the optical bandgap and a parameter that depends on the transition probability respectively. In above mentioned equation, exponent p depends on the type of transition. p may have values $\frac{1}{2}$, 2, $\frac{3}{2}$ and 3 corresponding to allowed direct, allowed indirect, forbidden direct and forbidden indirect transitions, respectively. The value of optical band gap has been taken as the intercept of extrapolation of $(\alpha hv)^{1/p}$ vs hv curve at $(\alpha hv)^{1/p} = 0$. The plot of Tauc, eq.(2), for a-GaTe thin film is shown in Fig. 3 and the obtained fitting

parameters B, E_g and p are given in Table 1. The optical bandgap is allowed direct type and is about 2.29 eV.



Fig. 3. Absorption coefficient (a) vs. photon energy (hv) for a-GaTe nanoparticles thin film. The circles represent the observed α and solid lines represent calculated α from: (a) Tauc model. (b) Urbach model.

Table 1. Fitting parameters from optical and electrical studies.

Sample	Tauc			Urbach		Activation energy (eV)	
	В	E _g (eV)	р	α	E ₀ (eV)	region I	region II
GaTe	3472.286±782.70	2.29 ± 0.374	0.469 ± 0.127	6358.64 ±35.810	$0.74{\pm}0.004$	0.314	0.834

In exponential edge region (where $\alpha < 10^4 \text{ cm}^{-1}$), in which the absorption depends exponentially on photon energy, Urbach relation [15] is obeyed:

$$\alpha h \nu = \alpha_0 \exp\left(\frac{h\nu}{E_0}\right) \tag{3}$$

where α_0 is a constant and E_0 is interpreted as band tail width of localized states, which generally represents the degree of disorder in amorphous semiconductors [16]. The plot of Urbach, eq.(3), for a-GaTe thin film is presented in inset of Fig. 3 and the obtained fitting parameters α_0 and E_0 are given in Table 1. The Urbach energy is found to be

about 0.74 eV. In this region, optical transitions take place between localized tail states and extended band states.

In weak absorption region ($\alpha < 10^2$ cm⁻¹), which involves low energy absorption, transitions originate due to defects and impurities.

3.3 Electrical studies

To know current transport mechanisms, the temperature dependent dc conductivity of a-GaTe nanoparticles thin films was measured in temperature range 345-525 K using two probes method. The dc conductivity of sample increases exponentially with increase in temperature indicating that conduction is through a thermally activated process which also shows the semiconducting behaviour of sample and is given by

$$\sigma_{dc} = \sigma_o \exp\left(\frac{-\Delta E}{kT}\right) \tag{4}$$

here ΔE is activation energy for dc conduction process, which is a function of electronic energy levels of chemically interacting atoms in the material and hence of energy band gap, and σ_o is pre-exponential factor which includes charge carrier mobility and density of states, k is Boltzmann constant, and T is absolute temperature. The plot of ln σ_{dc} vs. 1000/T for a-GaTe nanoparticles thin films is shown in Fig. 4. The plot shows two different temperature regions I and II. In region I, the increase in conductivity with temperature is attributed to variable range hopping in the localized states near the Fermi level. In this temperature region, there is no adequate number of charge carriers due to its intrinsic defects and the mobility of charge carriers is also low. In region II, the conductivity increases rapidly with increase in temperature. This behavior is due to the creation of more charge carriers with the increase of temperature. The low mobility of charge carriers is easily compensated by the creation of a large number of charge carriers and hence there is an increase in the conductivity of specimen [17]. The activation energies are calculated using eq.(4): in low temperature region, ΔE = 0.314 eV and in high temperature region $\Delta E = 0.834$ eV. The activation energy of thin film in the low-temperature region (below 406 K) is found to be smaller than that of the high-temperature region (above 406 K), confirming that conduction mechanism in low- and high-temperature regions is a thermally activated process and are known as variable range hopping in the localized states near the Fermi level; and thermally assisted tunneling of charge careers in the localized states near the band edges, respectively.



Fig. 4. Arrhenius plot of the dc conductivity of a-GaTe nanoparticles thin film.

4. Conclusions

a-GaTe nanoparticles thin films prepared by inert gas condensation technique has been checked as a nano-sized structure by XRD, SEM and FETEM analysis. These observations show that the prepared samples are amorphous, possess aggregates and have particle size in the range of 20–75 nm. The optical transition in the film has been found to be allowed direct having value ~ 2.29 eV. The Urbach energy, related to the width of band tail of localized states at conduction or valence band edge, has been determined and has the value ~ 0.74 eV. The dc electrical conductivity has been measured in temperature range 345–525 K. The calculated value of activation energy indicates that prepared samples behave as semiconductor material and the conduction is through a thermally activated process.

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