Superlattices and Microstructures 93 (2016) 1–10

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Structural and optical characterization of thermally evaporated bismuth and antimony films for photovoltaic applications

N. Srimathy, A. Ruban Kumar*

School of Advanced Sciences, VIT University, Vellore, 632014, India

ARTICLE INFO

Article history:
Received 6 October 2015
Received in revised form 11 February 2016
Accepted 17 February 2016
Available online 23 February 2016

Keywords:
Thermal evaporation
XRD
AFM
Raman spectroscopy
Sheet resistance

ABSTRACT

In this present study, the thin film of bismuth and antimony is coated by thermal evaporation system equipped with the inbuilt ultra high vacuum system. XRD analysis confirmed the rhombohedral structure of Bismuth and Antimony on the prepared film. The surface roughness and physical appearance is analyzed by Atomic force microscopy. The results of Raman Spectroscopy show the wave functions and the spectrum of electrons. The preparation technique and conditions strongly influence the crystalline structure and the phase composition of bismuth and antimony thin films. The electrical and optical properties for the prepared film are analyzed. The results show a great interest and promising applications in Photovoltaic devices.

1. Introduction

Thin film deposition technology, especially with vacuum deposition has greatly influenced the development of uniquely coated metallic thin films in recent decades. Each metal has their identical applications as per their physical and electronic properties. As the title implies, direct conversion of light into electricity without any interference of heat is known as Photovoltaic conversion. They do not require high maintenance and user–friendly for the generation of megawatts power. They find their applications in Building integrated PV, solar water pumping systems and even in space applications [1]. Especially, Bismuth and Antimony have generated much interest in photovoltaic applications due to their Photoelectric and reflective properties [2,3]. Literature shows that sulphides of antimony deposited by chemical deposition with less thickness provides *p*-absorber layer with optical band gap from 1.3 to 1.7 eV and with dark conductivity in the range of $10^{-3}\ \Omega\ cm^{-1}$ [2]. It is also reported that selenides of antimony have provided the dark conductivity in the range of $10^{-3}$to $10^{-4}\ \Omega\ cm^{-1}$ [3]. They are one of the most widely studied thermoelectric materials because of their distinctive features as they have long electron mean free path and small effective mass. Even though they differ fundamentally from classical semiconductors, these materials show a viable alternative because of their high reflectivity.

Bismuth and antimony materials are pentavalent metals which are identical to each other owing to their special properties, such as the significant reflectivity, surface resistance and roughness. They differ only in these peculiar features make their use in photovoltaic cells, concerning their highly anisotropic transport properties and high mobility of charge carriers. In

* Corresponding author.
E-mail address: arubankumar@vit.ac.in (A. Ruban Kumar).

http://dx.doi.org/10.1016/j.spmi.2016.02.026

the early years, researchers found that the variation of the electronic band structure of bulk material concerned their function of stoichiometry, temperature, strain, pressure, etc [4]. The high degree of anisotropy in their transport properties also distinguishes elements from other systems. A systematic study is required governing certain phenomena for the application in the field.

Both Bismuth and Antimony films grow with a perfect structure due to which there is an existence of high mobility of charge carriers. The possibility of developing these thin films with distinct structures exhibits both classical and quantum effects at different temperatures. It is also reported that reflectivity of the metals vary from near and far UV which can be better developed [5]. An absorber layer of thin film solar cells is the primary cause of the current voltage generation. The ionic radii and the band gap energy with its absorption coefficient match with its requirement in photovoltaic applications. Surface roughness is an important property in the electrochemistry of solid electrodes as the most of electric double layer and adsorption characteristics, as well as kinetic parameters are extensive quantities and referred to the apparent unit area at cross-section area of electrode surface [6]. The examination of the working area of solid electrodes is a difficult matter owing to the irregularities at a submicroscopic level for the determination of the real surface area of the solid electrodes.

The techniques and the conditions used for the film growth substantially affect the kinetic properties of the bulk properties. AFM study has presented great opportunities for the perfect study of the film structure. The present paper reports the results of AFM investigation of the structure of the Bismuth and Antimony films prepared through ultra-high vacuum thermal evaporation on glass substrates. AFM study reveals the presence of pure crystal of Bi and Sb films without any oxide and fluoride formation. It has seen from the X-Ray diffraction investigations that an ordered texture characterizes the crystal structure of Bismuth and Antimony films whereas, in the majority of cases, it is aligned perpendicular to the substrate plane. It has also shown that both the films from the crystallites with the decrease in substrate temperature.

As they have heavy mass, Bismuth films show that the optical phonon frequencies are low enough to display their scattering phenomenon by Raman Spectroscopy. The reflectance value always dependent on the thickness of the film coating. There will be a decrease in reflectance with the increase in film thickness. Their reflection profile was observed using UV-VIS spectrometer to expose their application towards solar technology to consider the cost effectiveness. Since Bismuth and Antimony are heavy metals by nature, they exhibit low optical phonon frequencies such that their oscillation periods are twice than 70 fs pulses [6]. The surface resistivity of the films is highly dependent on the surface temperature of the substrate and the deposition temperature. The thickness of the deposition shows their dependence in their characteristics as well.

In Photovoltaic applications, the films used in the deposition of cells or Anti-reflection or reflection coatings, the films may have unique Raman spectral shifts, and this can be used for their detection. The comparison of the properties of both Bismuth and Antimony gives in detail their wide application in photovoltaic which is presented in this analysis.

2. Experimental setup

Several techniques for thin film deposition were used for the cell preparation of photovoltaic applications. The deposition procedure and the thickness of both bismuth and antimony were maintained to compare their characteristics. Thin films of bismuth and antimony deposited in thermal evaporation system inbuilt with Ultra high vacuum system. The source and the substrate temperature was maintained the same for both the deposition. The Evaporation system was initially evacuated down to a base pressure of 1×10^{-6} Torr by high vacuum pumps. Spectroscopically pure bismuth and antimony (99.999% of purity) were used as the source material in the Molybdenum boat for the deposition. The substrates were cleaned by Ultrasonic method of cleaning with Reozonized water. Glass substrates of dimension 100 mm $\times$ 100 mm loaded in the chamber. A calibrated and welded (chromel-alumel) thermocouple was used for measuring the substrate temperature. The substrate temperature was maintained at 30° C.

In the beginning, pure bismuth was evaporated from a molybdenum boat. Initially, the system was evacuated to a high vacuum, and the substrates were subjected to the ionic bombardment for 10 min in the vacuum chamber before the deposition of the film. Throughout the deposition process, the rate of evaporation was maintained within the range of 10–15 nm/min. After 20 min of deposition, the substrate was removed safely from the system.

The thickness of the film was measured and controlled using the quartz crystal thickness monitor and also checked again by dektak Thickness profiler. Secondly, antimony was loaded in the same molybdenum boat, and same deposition techniques maintained. A thickness of 200 nm deposited over a period for 20 min. Since there is a difference in their melting points, the heaters connected to the boat were set accordingly to the melting point of the materials to be deposited. Film sheet resistance was also measured using a four-probe set-up. Silver epoxy used as ohmic contacts for the accurate measurement.

The comparison of their properties for their applications in energy field can assure by analyzing their behavior by the following characterization techniques, namely thickness and sheet resistance measurement, X-ray diffraction (XRD, Brucker D8 Advance, Cu Kα radiation, $\lambda = 1.5406$ Å) with a range of 2θ from 10° to 80° operated with 40 kV and 10 mA Atomic Force Microscopy (AFM, Veeco Dimension V), Raman Spectroscopy (Seiki Tecnotron), Shimadzu UV–VIS spectrometer with 1 nm resolution at a scan speed of 240 nm/min.

The results obtained by the above characterization tools helps in the analysis of their difference in structural and optical properties.