Grown of InTe films by close spaced vapor transport

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InTe films were grown on glass substrates by close spaced vapor transport (CSVT) using evaporation of In_2Te_3. The composition of the films was investigated by Auger electron spectroscopy. The InTe films were investigated by X-ray diffraction using bragg-Bentano method. The application of the rietveld refinement patterns provides information about the crystallographic structure, lattice constants, atomic positions and bond lengths of the films. Optical characterization by Raman spectroscopy gave us further evidence of the success in the production of InTe films.

*Keywords:*Indium Telluride; Semiconductors; X-ray diffraction; Raman spectroscopy

1. Introduction

Indium telluride is a III-VI semiconducting compound with a chain TlSe-type structure and it has a potential to be used for photovoltaic device applications. The structure of InTe compound can be described by the formula $In^{+}In^{3+}Te^{2-}{}_2$. Under ambient conditions it crystallizes with the space group I4/mcm [1, 2]. In^{3+} ions are tetrahedrally coordinated to Te^{2-} ions whereas In^{+} ions have 8-fold tetragonal antiprismatic coordination by Te^{2-} ions. The chemically distinct In^{3+} and In^{+} ions occupy two different crystallographic positions preventing free transfer of electrons from the In^{+} to the In^{3+} [3]. The growth of InTe films have been reported previously [4, 5, 6], in all cases they were evaporated from InTe material using flash evaporation technique. Close-spaced vapor transport is a convenient method for growing semiconductor materials because its simplicity, moderate processing temperature, high transport efficiencies of the source material, and ability to be easily scaled up to high-volume continuous processing. It is also cost-effective as it can operate at atmospheric pressure under inert gas and uses moderate temperatures; its operation is simple, and films are compact with few voids. In this work the growth of InTe films by close spaced vapor transport is reported. Also, we characterized the InTe films by X-ray diffraction (XRD), Auger and Raman spectroscopies. All the results give irrefutable evidence of the production of polycrystalline InTe films.

2. Experimental details

All films were prepared in a conventional vacuum with

Table 1. Unit cell parameters, interatomic distances (Å) and bonding angles (degrees) of InTe film.

Space group	**I4/mcm**
Lattice parameters	
a(Å)	8.4522(3)
b(Å)	8.4522(3)
c(Å)	7.1327(2)
V(Å^3)	509.56(1)
Interatomic distances (Å)	
In(1)-Te	2.81994(5)
In(2)-Te	3.57153(5)
Bonding angles	
In(1)-Te-In(2)	78.447(2)
Te-In(1)-Te	101.553(2)
Te-In(1)-Te	113.569(1)
Te-In(2)-Te	75.579(2)

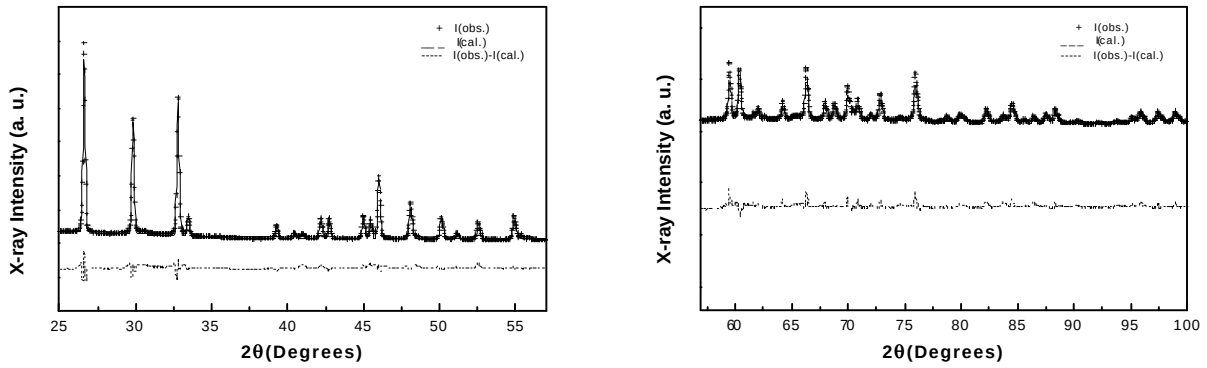

Figure 1. Rietveld refined profile of X-ray diffraction data for a representative InTe film (a) range 25 to 55 degrees, (b) range 55 to 100 degrees.

an evaporation system evacuated by an oil-diffusion pump liquid-nitrogen trap, capable of obtaining a background pressure of 10^{-6} Torr. The pressure during evaporation was below 10^{-5} Torr. The CSVT apparatus used has been described previously [7]. The raw material In_2Te_3 99.999 at. % from Balzers. Corning 7059 glass slides were used as substrates. The In_2Te_3 source was maintained at 825 °C during the growth process. We kept fixed the substrate temperature at 400°C, and the deposition time at 10 min. Elemental concentrations were determined by Auger electron spectroscopy (AES) using a Perkin-Elmer PHI-560 ESCA-SAM, the Auger spectra were obtained after 7 minutes of Ar+ sputtering employing a beam energy of 4 keV. X-ray diffraction measurements were performed with a Rigaku rotative anode X-ray generator,Geigerflex diffractometer CuKα radiation, 40 KV, 40mA, set scanning mode, step 0.02 degrees, scan time 8 seg. The experimental XRD data were analyzed by the Rietveld profile fitting procedure using the GSAS program [8]. Room temperature Raman experiments were carried out in a Labram Dilor micro Raman system employing a HeNe laser.

3. Results and discussion

The surfaces of the films were smooth and slightly grayish. All the films were firmly adhered to the substrate. The films are polycrystalline, with uniform thickness (around 25 μm). The XRD patterns of the polycrystalline films indicate the features of InTe single phase material. The basis for indexing the diffractogram was the tetragonal lattice with a=8.444 Å, c=7.136 Å [9]. The analysis of the crystal structure of InTe was done with the I4/mcm group. The structure factors were calculated using the atomic scattering factors of In and Te. The background was fitted with a polynomial function. The half-with and asymmetry parameters for the peak shape, scale factor, positional and isotropic thermal parameters for all atoms, unit cell parameters and preferred orientation were refined. The XRD intensities were corrected for pseudo-Voigt function. The final refinement cycle carried out yielded the conventional reliability factors R_{bragg}=13.7, W_{Rp}=12.6 and R_p=9.8 [10]. The results are listed in Table 1. The refined parameters of atomic coordinates are listed in Table 2. The structure contains two different In atoms sites. In(2) atoms are surrounded of eight Te atoms, with In-Te distances of 3.57153(5) (Å). In(2) atoms can be thought to be in the In^+ state. In(1) atoms are in In^{3+} state and are covalently bonded to four Te atoms with In-Te bond distances of 2.81994(5) (Å). Figure 1a and 1b shows the observed and calculated X-ray diffraction profiles and their differences after the refinement. The good fitting gives evidence that our films are InTe. In fact, the values obtained after the refinement are in agreement with the reported on ICSD (Inorganically Crystal Structure Database) and PDF (Powder Diffraction File) card 300636.

Figure 2 shows the Auger spectrum for representative sample only for the region were signal was obtained, and it clearly shows that the film consisted only of indium and telluride. The ratio of the peak-to-peak intensities among indium and telluride peaks taking in account the sensitivity factors of S_{Te}=1 and S_{In}=1.76; indicated roughly that the film has the right composition of InTe.

Table 2. Atomic coordinates of InTe film

Atom	Wyckhoff	x	y	z	Occ.
In(1)	4a	0	0.5000(2)	0.2500(2)	1
In(2)	4b	0	0	0.2500(2)	1
Te	8h	0.1824(1)	0.6821(2)	0	1

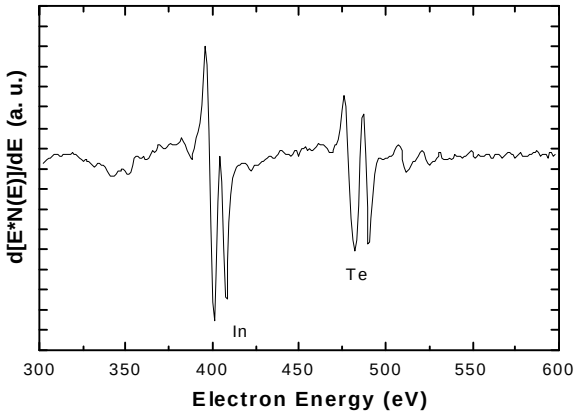

Figure 2. Auger electron spectroscopy results obtained for representative InTe sample.

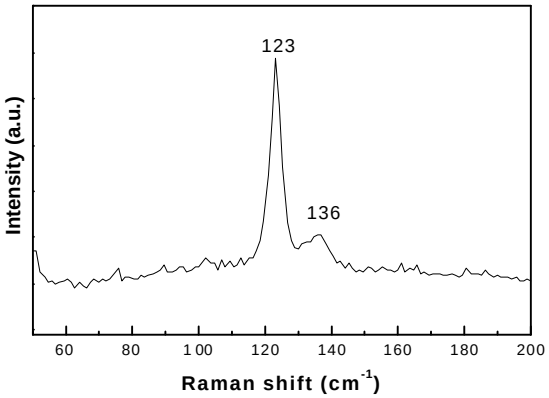

Figure 3. Raman spectrum of representative InTe sample.

Raman spectroscopy is a well established technique very sensitive to the microscopic atomic arrangement. Figure 3 shows the Raman spectrum obtained for representative sample . It revealed two structures, with peaks around 123 and 136 cm^{-1}, in agreement with previous Raman measurements reported for InTe single crystal material [11].

4. Conclusions

In summary, the results of XRD indicated that the films grown by CSVT were single phase InTe films. Raman spectroscopy and AES measurements demostrated that the grown films were InTe. Although the detailed studies of the grown mechanism of the films were not fully understood, these InTe films grown on glass substrates by CSVT might lead to interesting device applications.

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