

Local structure and physical properties of In_3SbTe_2 : Characterizing a member of a fourth family of phase change materials

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Abstract

We report on the structure and physical properties of the In_3SbTe_2 phase change material. This compound has a stoichiometry that deviates significantly from other phase change materials such as alloys on the pseudo-binary line between GeTe and Sb_2Te_3 , doped Sb or doped Sb_2Te . Hence In_3SbTe_2 belongs to a fourth family of phase change materials. Yet, it shows many similarities with other phase change alloys such as an octahedral-like atomic arrangement, fast crystallization and property contrast between the amorphous and crystalline state. In this study, a systematic comparison with other phase change alloys is presented and the measured properties of In_3SbTe_2 will be discussed employing ab-initio calculations.

Key words: Structural properties, resonance bonding, InSbTe, PCM families.

1. Introduction

Phase change materials have advanced significantly in the last decade. Nevertheless there is still a need to improve several properties for specific applications.^{1,2} Hence a systematic understanding of the properties of phase change materials is highly desirable. So far, studies have focused on three different families of materials. Alloys on the pseudo-binary line between GeTe and Sb_2Te_3 , doped Sb and doped Sb_2Te form three families of phase change materials with similar properties.² Interestingly, $\text{In}_3\text{Sb}_1\text{Te}_2$ deviates significantly from the stoichiometry of the phase change materials identified so far. InSbTe alloys were already characterized for application in optical data storage. They reveal erase times of < 50 ns and an endurance of 10^5 write cycles.³ Recently, this material was also investigated for multilevel electronic storage.³ Here we present a systematic study of the structure and physical properties of In_3SbTe_2 .

2. Experiments

In_3SbTe_2 (IST) thin films are d.c. sputter-deposited from a single IST target of 99.99% purity. Measurements such as electrical sheet resistance and grazing incidence x-ray diffraction (GI-XRD) are performed on thin films (74.0 ± 0.1 nm). The extended x-ray absorption fine structure (EXAFS) has been measured at liquid Helium temperature for all three K absorption edges of crystalline IST.

3. Results and discussion

Figure 1a displays the comparison of the electrical properties of IST with GeTe and GeSb_2Te_4 .⁴ IST has a higher resistance in the amorphous state and a lower resistance in the crystalline phase as compared with both GeTe and GeSb_2Te_4 . In addition, IST has a significantly higher crystallization temperature. Figure 1b depicts a pronounced dependence of crystallization temperature on film thickness, which could be interesting for scaling.

Figure 2 presents structural analysis by grazing incidence x-ray diffraction on IST thin films annealed at different temperatures. As-deposited films remain amorphous up to an annealing temperature of 200 °C. Around 220 °C, the films start to crystallize into a single IST phase. This cubic phase (lattice constant 'a' = 6.106 ± 0.005 Å) remains stable up to 325 °C. Additional

confirmation of the local atomic environment of crystalline IST by EXAFS reveals the majority (> 95 %) of all three types of atoms to be arranged in an octahedral-like arrangement with a nearest neighbor spacing as shown in table1. In addition, there is evidence for a small segregation of InSb (see fig. 3). 5 (\pm 1) % of the atoms are likely to form crystalline InSb. A quantitative analysis leads to further information on the local structure of the rock-salt like phase and all atomic distances found for the IST phase are summarized in Table 1.

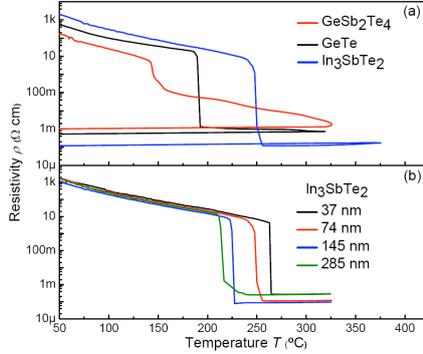


Figure 1: (a) Temperature dependent resistivity of IST, GeTe₂Sb₄, GeTe films. (b) Thickness dependent resistivity of IST thin films.

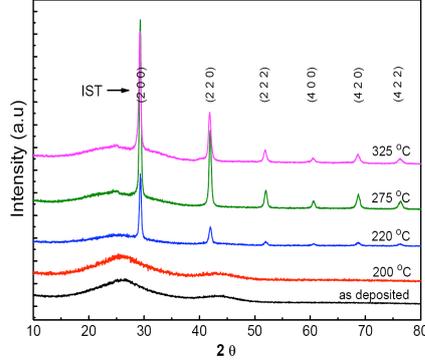


Figure 2: Temperature dependent GI-XRD measurement on IST thin films.

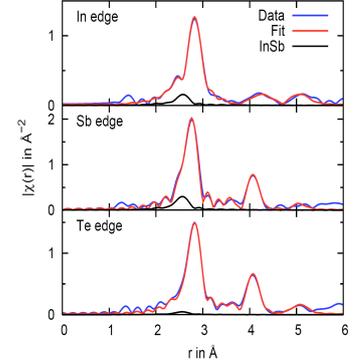


Figure 3: Fourier transformed EXAFS data of crystallized IST (blue) with total fit (red) and contribution from segregated InSb (black).

In edge [$S_0^2=0.66(2)$, $R=0.005$]		
Bond type	Distance	MSRD
In-Sb	2.99(1) \AA	0.0025(3) \AA^2
In-Te	3.07(2) \AA	0.0032(2) \AA^2
Sb edge [$S_0^2=0.65(4)$, $R=0.010$]		
Sb-In	2.99(1) \AA	0.0025(3) \AA^2
Te edge [$S_0^2=0.60(2)$, $R=0.011$]		
Te-In	3.07(2) \AA	0.0032(2) \AA^2

Table 1: Atomic distances and Mean Squared Relative Displacements (MSRD) in the rock-salt-like phase of crystallized IST.

Material	$T_{\text{ann.}}$ ($^\circ\text{C}$)	σ_{vap} S.cm^{-1}	$\sigma_{\text{opt.}}$ S.cm^{-1}	$n \times 10^{20} \text{cm}^{-3}$	$\mu \text{cm}^2/\text{Vs}$
GeTe	250	2074	1339	5.7	22.5
GST124	200	10.1	52	1.2	0.5
GST124	300	794	711	2.2	22.6
Sb ₂ Te	250	-	2500	8.8	11.66
AIST	240	-	1770	17.3	6.1
GIST	240	-	2970	29.2	6.5
In ₃ SbTe ₂	250	9320	12086	168	3.53
Sb	200	3030	~	3.6	53

Table 2: Comparisons of transport properties of various crystalline phase change materials.

A comparison of electrical and optical properties of IST with other phase change alloys is summarized in table2. The electrical conductivity and the carrier concentration of the crystalline IST is almost one order of magnitude larger than that of the other phase change materials. This is in line with the smaller average number of p-electrons of IST.

4. Conclusion

IST has a stoichiometry which significantly deviates from the three other families of phase change materials. This member of a fourth family of phase change alloys displays an excellent thermal stability and an octahedral-like atomic arrangement.

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