E*PCOS2010

Local structure of amorphous $Ge_8Sb_2Te_{11}$

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ABSTRACT

We report on a study of the local structure of as-deposited amorphous $Ge_8Sb_2Te_{11}$ over the temperature range from 10 K to 400 K. We demonstrate that the structure consists of a complex mixture of Ge-Ge (2.47 Å), Ge-Te (2.6 Å), Ge-Sb (2.68 Å), Sb-Te (2.83 Å) bonds satisfying the 8-N rule. All bond lengths increase with increasing temperature. The Einstein temperature is higher for shorter bonds.

Keywords: Ge-Sb-Te, local structure, EXAFS

INTRODUCTION

One of the ways to satisfy the need for larger storage densities [1], is to reduce the size of the encoding mark. This can be achieved using shorter wavelength lasers and higher numerical aperture lens such as 405 nm and 0.85, respectively in the case of the Blu-Ray disc technology. At the same time memory devices call for a stable amorphous phase and a high optical contrast between the crystalline and amorphous states in the blue-violet spectral region. GeTe-rich Ge-Sb-Te alloys meet these demands. In order to futher optimize the encoding process, a knowledge of the structure of both phases which determine their physical-chemical properties is a crucial.

In this work, we report on observations of the local order in an as-deposited $Ge_8Sb_2Te_{11}$ composition, designed for the Blu-Ray disc technology [2], over the temperature range from 10 K to 400 K.

EXPERIMENTAL DETAILS

A $Ge_8Sb_2Te_{11}$ film was deposited using RF magnetron sputtering on both sides of an aluminum foil substrate. The thickness of the deposited film was about 2 μm. Subsequently, the sample was cut into small pieces (approximately 8×8 mm) and stacked to a thickness optimized to achieve a x-ray absorption edge step of unity for each element. The EXAFS measurements were performed over the temperature range from 10K to 400 K at the BL14B2 beamline at the Japan Synchrotron Radiation Research Institute (SPring 8). Collected data were analysed using program packages Athena and Artemis [3].

RESULTS & DISCUSSION

The real parts of χ(R) for the Ge, Sb and Te K edges of the as-deposited $Ge_8Sb_2Te_{11}$ are displayed in Fig. 1(a) together with fits to the data. The robustness of the model selection and undesirable data correlations were minimized using both single and multi edge fitting. In our model, the Ge edge first coordination shell χ data could be fit using three backscattering paths Ge-Ge, Ge-Sb and Ge-Te , Te edge χ data could be fit using two backscattering paths Te-Ge and Te-Sb and Sb edge χ data could be fit using two backscattering paths Sb-Ge and Sb-Te. The passive electron reduction factor $S_0{}^2$ was fixed to a value of 0.8. The set of applied backscattering paths is in a good agreement with those used in works [4, 5] Our obtained data are different from those acquired from the molecular dynamic simulation [6] The fitting parameters are summarized in the table1. The total coordination numbers for each element ($N_{Ge} = 3.8$, $N_{Sb} = 3.04$ and $N_{Te} = 2.01$) were consistent with the 8-N rule.

In the EXAFS equation, disorder is expressed by the mean square relative displacement (MSRD) which is related to the bond vibrations and is thermally dependent. The temperature dependence of the bond strength can be well approximated by the correlated Einstein model where the projected density of vibrational states is approximated by a single mode at frequency $\omega_E = \frac{\Theta_E k_b}{\hbar}$ where Θ_E is the Einstein temperature. The obtained data were fit using the Einstein model according to the formula:

$$\Delta\sigma^2_{TH}(\Theta_E, T) = \frac{\hbar^2}{2\mu k_R \Theta_E} \coth\left(\frac{\Theta_E}{2T}\right) + \sigma_0^2 \quad (1)$$

where T is the absolute temperature, μ is the reduced mass of the pair of atoms forming bonds and $\sigma_0{}^2$ represents static disorder. It is clear from Fig. 1 and the Table 1 that the Einstein temperatures of atoms bonded to Ge (Ge-X) bonds are higher and therefore these bonds are stiffer than Sb-Te bonds. The bond strength of Ge-X bonds is larger for shorter bonds.

Table 1: Scattering paths that were used at all edges. The first atom represents the absorber and the following one is the backscatterer. N describes the coordination number of the absorbing atoms, r represents the bond length and θ_E is the Einstein temperature.

	Ge-Ge	Ge-Te	Te-Ge	Ge-Sb	Sb-Ge	Sb-Te	Te-Sb
N	1.34±0.2	2.18±0.15	1.64±0.1	0.28±0.1	1.24±0.1	1.8±0.2	0.37±0.1
r (Å)	2.47±0.01	2.6±0.01		2.68±0.01		2.83±0.01	
Θ_E (K)	342±9%	320±5%		300±5%		225±3%	

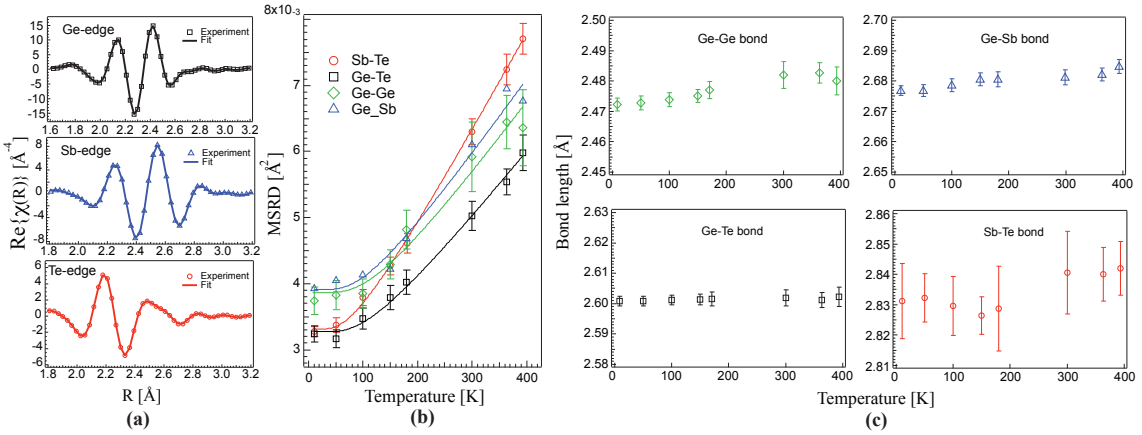

Figure 1. a) The real parts of χ(R) of the Ge, Sb and Te K edges of the as-deposited $Ge_8Sb_2Te_{11}$ (open rings) at 10 K and the respective fits b) MSRD as a function of temperature in the amorphous film of $Ge_8Sb_2Te_{11}$. Sb-Te bond : open red ring, Ge-Te bond : open black square, Ge-Ge bond: open green rhombus and Ge-Sb bond: open blue triangle. c) The bond length thermal dependence of Ge-Ge, Ge-Te, Sb-Te and Ge-Sb bonds.

CONCLUSION

The bonding in as-deposited $Ge_8Sb_2Te_{11}$ has a covalent character with total coordination numbers ($N_{Ge} = 3.8$, $N_{Sb} = 3.04$ and $N_{Te} = 2.01$) that satisfies the 8-N rule. The bond lengths obtained were 2.47 Å for Ge-Ge bonds, 2.6 Å for Ge-Te bonds, 2.68 Å for Ge-Sb bonds and 2.83 Å for Sb-Te bond. The bond strength of Ge-X bonds increases for shorter bonds. Ge-X bonds are stiffer than Sb-Te bond.

MK gratefully acknowledges JSPS for his research fellowship. We also thank to SPring8 proposals 2009B1206 and ..... for the financial support.

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