

Article

Study on Texture Formation of Sb₂Te Thin Films for Phase Change Memory Applications

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Abstract: We investigated the texture formation of Sb₂Te thin films for phase change memory applications. The Sb₂Te thin films with different thicknesses were deposited on Si (100) wafers by the magnetron sputtering method. As-deposited Sb₂Te thin films were annealed at various temperatures and times. The texture characterization was performed by using X-ray diffraction (XRD) and electron backscatter diffraction (EBSD). Experimental results show that the annealed Sb₂Te thin films exhibit the {11 $\bar{2}$ 0} and {10 $\bar{1}$ 0} prismatic texture. The formation of prismatic texture is induced by the lattice strain, surface energy, and coarse grains, in which the lattice strain is the essential origin of prismatic preference. Electronic transport properties of Sb₂Te thin films were monitored by a physical property measurement system (PPMS). It was found that the formation of prismatic texture promotes the increase of carrier mobility. The stability of the film–substrate interface was also assessed by calculating mismatch. The prismatic-preferred Sb₂Te thin films exhibit higher mismatch with a silicon wafer, reducing the interface stability.

Keywords: phase change memory; Sb₂Te thin films; prismatic texture; electrical properties; interface stability



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1. Introduction

Phase change memory (PCM) is one of the most promising contenders for next-generation nonvolatile memory [1–3]. The data writing, erasing, and reading rely on the switching of PCM between a high resistance state (RESET state) and a low resistance state (SET state) that is operated by a rapid electrical pulse at a nanosecond scale. Nonvolatility, scalability, and compatibility with the CMOS (complementary metal oxide semiconductor) technique make PCM useable in commercial embedded chips. More challenging scenarios, such as terminal display [4], memory computing [5], and artificial neurons [6], propose requirements for PCM device performance. (1) Data switching should be completed rapidly to provide high-speed processor operation and system response. (2) Sustainability is needed to resist density change and composition deviation induced by long-term cycling. (3) Reduced power consumption is necessary for the future green industry, in which a lower electrical pulse is applied to overcome the switching energy barrier. The key to the PCM device is a nanoscale chalcogenide compound, which is also called PCM thin film. The structural and physical properties of the PCM thin film strongly depend on the component and microstructure features, which in turn impact the switching performance of the PCM device. Therefore, microstructure investigation and component development of PCM thin film has come to the center of attention.

Crystallographic orientation optimization has attracted interest in polycrystalline PCM thin films. As suggested by Behera et al. [7], transport properties are related to texture intensity. PCM thin film with adjustable texture is desirable to explore potential opto-electrical properties. Ie et al. [8] prepared basal preferred Ge₂Sb₂Te₅ thin film by using multilayer deposition and modulating constituent methods. Experimental results showed that the resistances of as-deposited and textured Ge₂Sb₂Te₅ thin films are 14.75 kOhm/cm² and

5.45 Ohm/cm², respectively, satisfying the requirements of the electrical signal difference. Simpson et al. [9] prepared a highly orientated GeTe thin film along the [001] direction that exhibits the optimized crystallization time and activation energy. In highly orientated PCM thin films, texture formation confines the movement of the atoms to decrease the entropy losses, allowing a lower activation energy and faster switching operation [10]. That is to say, orientation preference has an impact on the phase transition mechanisms and data conversion characteristics. It suggests that texture is the controllable parameter to tune microstructure and optimize properties of PCM thin film.

Sb₂Te thin film, an advanced Sb–Te binary PCM system, has gained attention. Sb₂Te has a simple composition and stable phase [11]. Moreover, the crystallization of Sb₂Te thin film is dominated by grain growth, which could realize high-speed phase transition [12]. PCM device based on Sb₂Te thin film could complete data conversion within 20 ns [13], being compatible with the rapid response of the system. Lower power consumption and higher retention stability are expected in challenging occasions, which are linked to the improvement of the physical properties of Sb₂Te thin film. The texture is a degree of freedom to tailor the properties of Sb₂Te thin film. Nevertheless, little is known about the orientation preference of Sb₂Te thin film. The texture formation mechanism is discussed less often. The correlation between crystallographic orientation and physical properties still has to be examined to promote appealing applications of Sb₂Te thin films.

Inspired by this topic, we studied the texture of Sb₂Te thin films for phase change memory applications. First of all, by employing the XRD and EBSD, the texture of Sb₂Te thin films annealed at various temperatures was characterized. Next, by designing and fabricating the 200 nm and 1000 nm Sb₂Te thin films annealed at various times, the formation mechanism of prismatic texture was investigated. Finally, the electronic transport properties of Sb₂Te thin films with prismatic texture were explored. The stability of prismatic-preferred Sb₂Te thin films was also analyzed. We suggested that reducing the prismatic texture intensity is beneficial to improve the resistance and interface stability of the Sb₂Te thin films.

2. Materials and Methods

2.1. Sample Preparation

Sb₂Te thin films with ~200 nm were deposited on the Si (100) wafers using a direct current (DC) magnetron sputtering method. The single stoichiometric Sb₂Te target was employed. The background pressure in the deposition chamber was lower than 1×10^{-5} torr. The argon flow was set to 33 sccm and the argon pressure was 5×10^{-3} torr. To ensure the deposition homogenization, the rotation substrate was utilized. The film composition was verified by the ZEISS Merlin Compact field emission scanning electron microscope (FE-SEM) equipped with energy dispersive spectroscopy (EDS). To study the texture formation mechanism, the Sb₂Te thin film with ~1000 nm was deposited by extending the sputtering time. The as-deposited Sb₂Te thin films were annealed in the vacuum chamber to obtain the crystalline states.

2.2. Texture Characterization

A Bruker D8 Advance X-ray diffractometer (XRD) was employed to characterize the phase structure and measure the pole figures (PFs). Cu K α X-ray ($\lambda \sim 0.154$ nm) was used. When the phase structure was detected, the scan range was $2\theta = 20^\circ \sim 80^\circ$. The lattice parameters were calculated by Jade 5 software. The $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ PFs were measured using the Schulz method with Eulerian cradle. The range of the φ angle was $0^\circ \sim 360^\circ$, and the range of the χ angle was $0^\circ \sim 70^\circ$. The scan step was 5° . The grain orientation characterization was conducted by using electron backscatter diffraction (EBSD). The $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs were calculated to assess texture intensity by employing TSL OIM Analysis 8 software.

An FEI Tecnai F20 transmission electron microscope (TEM) was used to perform the microstructure characterization. Micromorphology and high-resolution phase con-

trast (HRTEM) images were captured. Inverse fast Fourier transform (IFFT) images were calculated by using Gatan Digital Micrograph 3 software to verify the phase stability.

2.3. Electrical Property Measurement

The carrier mobility and carrier density were measured by employing a Quantum Design PPMS-9 physical property measurement system. The van der Pauw (vdP) method was used. The detection area was $8 \times 8 \text{ mm}^2$. Two random regions were tested to improve the reproducibility of measurements.

2.4. Interface Mismatch Calculation

In order to discuss the role of texture in the stability of Sb_2Te thin film, an edge-to-edge matching (E2EM) model [14,15] was used to calculate the mismatch of the thin film–silicon wafer interface.

3. Results

3.1. Texture Characterization of Sb_2Te Thin Films

Figure 1 shows XRD patterns of Sb_2Te thin films annealed at various temperatures. After annealing at 140°C , the amorphous diffraction peak could still be observed at $\sim 29.2^\circ$. It suggests that the as-deposited Sb_2Te thin film is in amorphous state. Only one weak crystallographic diffraction peak appears at $\sim 42.1^\circ$, which corresponds to the $\{11\bar{2}0\}$ plane of Sb_2Te thin film, as displayed in Figure 1a. It indicates that the crystallization temperature of Sb_2Te thin film is $\geq 140^\circ\text{C}$, and the Sb_2Te thin film annealed at 140°C is not fully crystallized. A broad peak is found at $\sim 69.3^\circ$, which is related to Si substrate, consistent with reference [16]. As shown in Figure 1b, when the Sb_2Te thin film is annealed at 200°C , the amorphous diffraction peak vanishes. A sharp $\{11\bar{2}0\}$ diffraction peak emerges. Meanwhile, another strong peak could be observed that originates from $\{30\bar{3}0\}$ plane diffraction. Moreover, the weak diffraction peaks appearing at smaller angles ($\sim 28.6^\circ$ and $\sim 39.5^\circ$) are associated with $\{10\bar{1}3\}$ and $\{01\bar{1}6\}$ crystal planes. It implies that the amorphous Sb_2Te thin film is transformed into a crystalline state, and the $\{11\bar{2}0\}$ oriented grains exert preferential growth. As the annealing temperature increases to 400°C (Figure 1c), the peak intensities of $\{11\bar{2}0\}$, $\{30\bar{3}0\}$, $\{10\bar{1}3\}$, and $\{01\bar{1}6\}$ planes are strengthened. It indicates the increase of crystallization fraction of Sb_2Te thin film with the increased temperature. No diffraction peaks of other phases are found in the XRD patterns, indicating the stability of Sb_2Te lattice. In addition, the $\{11\bar{2}0\}$ oriented diffraction peaks with higher intensity may result from the strong $\{11\bar{2}0\}$ texture.

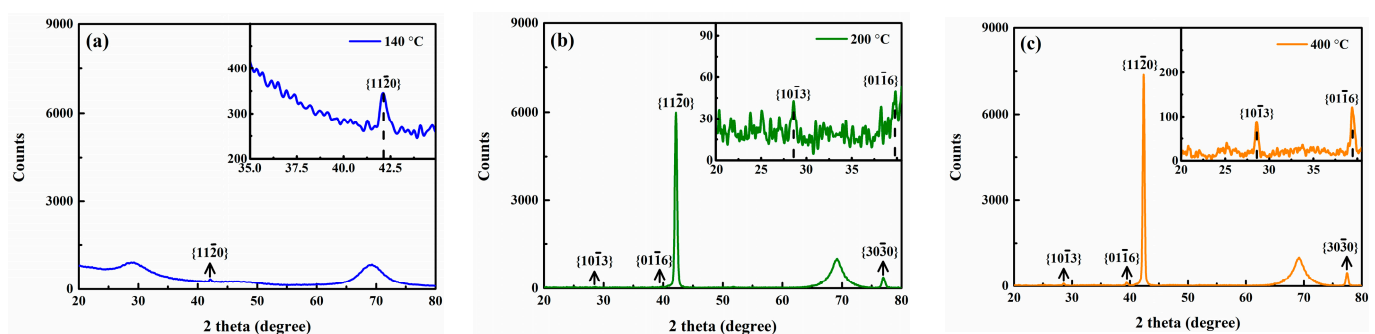


Figure 1. XRD patterns of Sb_2Te thin films (200 nm) annealed at different temperatures: (a) 140°C ; (b) 200°C ; (c) 400°C . The holding time is 30 min. The inset in (a) is an enlarged diffraction signal between 35.0° and 44.9° . The inset in (c) is a redrawn diffraction signal between 20.0° and 40.5° .

Figure 2 shows the $\{11\bar{2}0\}$ PFs of Sb_2Te thin film measured by XRD. As displayed in Figure 2a, when the annealing temperature is 140 °C, the maximum pole intensity of $\{11\bar{2}0\}$ PF is 1.2. With the enhanced annealing temperature (see Figure 2b,c), the maximum pole intensities increase to 3.6 (200 °C) and 4.4 (400 °C), respectively. In the measured $\{11\bar{2}0\}$ PF, the corresponding pole sites are located near the center of the PF. When the pole density is higher than 1, distribution of pole sites deviates from randomization, indicating the existence of $\{11\bar{2}0\}$ orientation preference. The higher the pole density, the stronger the texture intensity. The results show that the $\{11\bar{2}0\}$ pole density increases with the increase of annealing temperature. That is to say, Sb_2Te thin films annealed at various temperatures possess the $\{11\bar{2}0\}$ texture, being compatible with the results of XRD patterns.

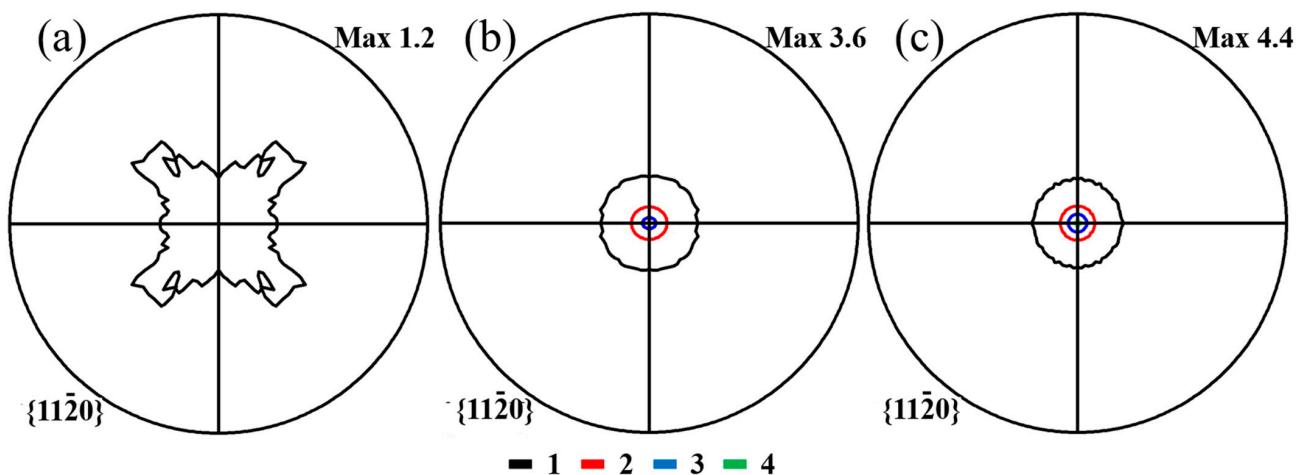


Figure 2. Measured $\{11\bar{2}0\}$ PFs by XRD for Sb_2Te thin films (200 nm) annealed at (a) 140 °C; (b) 200 °C; (c) 400 °C. The holding time is 30 min. Different colors represent pole density levels: black for 1, red for 2, blue for 3, and green for 4. The green curve is a small circle at the center of (c). The maximum pole density is near the center of the measured PFs.

Figure 3 shows the crystallographic orientation mapping images and calculated $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs of Sb_2Te thin films annealed at 140 °C, 200 °C, and 400 °C. In orientation maps (Figure 3a–c), grains colored by red represent $\{0001\}$ basal parallel to the thin film surface. The grains are marked in blue and green and possess $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ prismatic orientation. The $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ orientated grains dominate in Sb_2Te thin film, indicating the formation of a sharp prismatic texture.

Figure 3d–g show the calculated $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs. Maximum pole intensities are around the center of the calculated $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs, consistent with PFs measured by XRD. It indicates that the density of other orientation is weaker in Sb_2Te thin film. After annealing at 200 °C, the maximum pole densities in the $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs are 6.314 and 5.382. When the annealing temperature elevates to 400 °C, maximum intensities for $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs increase to 7.162 and 7.089. Therefore, the prismatic texture is formed and maintained in Sb_2Te thin film.

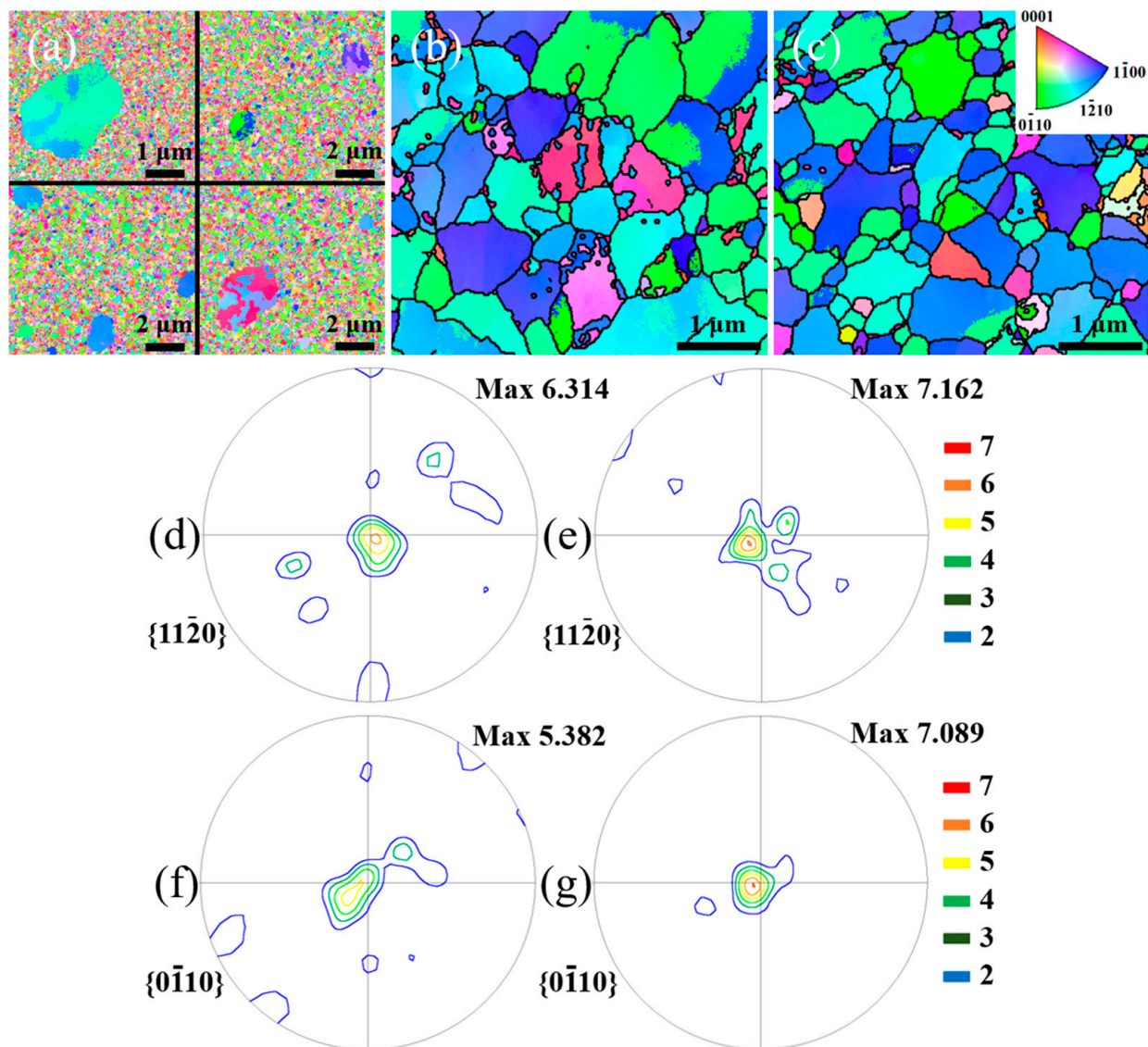


Figure 3. Orientation mapping images of Sb_2Te thin films (200 nm) annealed at different temperatures: (a) 140 °C; (b) 200 °C; (c) 400 °C. The holding time is 30 min. Calculated $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ PFs counted from EBSD maps of Sb_2Te thin films annealed at (d,f) 200 °C; (e,g) 400 °C. Panel (a) shows the four randomly captured crystallized regions. Different colors represent pole density levels: blue for 2, dark green for 3, light green for 4, yellow for 5, orange for 6, and red for 7. The maximum pole density is near the center of the calculated PFs.

3.2. Formation Mechanism of Prismatic Texture

The previous results show the strong diffraction peaks of $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ planes in XRD patterns, numerous grains with $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ orientation in EBSD mappings, and high $\{11\bar{2}0\}$ and $\{01\bar{1}0\}$ pole densities in PFs. These suggest that Sb_2Te thin films exhibit $\{11\bar{2}0\}$ and $\{10\bar{1}0\}$ prismatic texture. The orientation preference may be dictated by the phase transformation, surface energy minimization, and strain energy minimization. The inheritance of texture caused by the phase transition in alloys has been confirmed [17,18]. Phase separation leads to inhomogeneous composition, which may be the cause of orientation preference. Phase stability of Sb_2Te thin film was considered firstly. XRD and EBSD analyses revealed the phase stability at the relative macro scale. TEM was utilized to observe the microstructure and lattice stability of Sb_2Te thin film at the microscale. Figure 4a,c,e show the microstructure of Sb_2Te thin films annealed at 140 °C, 200 °C, and 400 °C. The second phase precipitation is not observed. We captured

the high-resolution phase contrast (HRTEM) images of lattices and grain boundaries (GBs) in Sb_2Te thin film, and the inverse fast Fourier transform (IFFT) images were calculated. As shown in Figure 4b,d,f, several crystal planes of Sb_2Te are indexed. It demonstrates the phase stability of Sb_2Te thin films at different temperatures, in agreement with the results of XRD and EBSD.

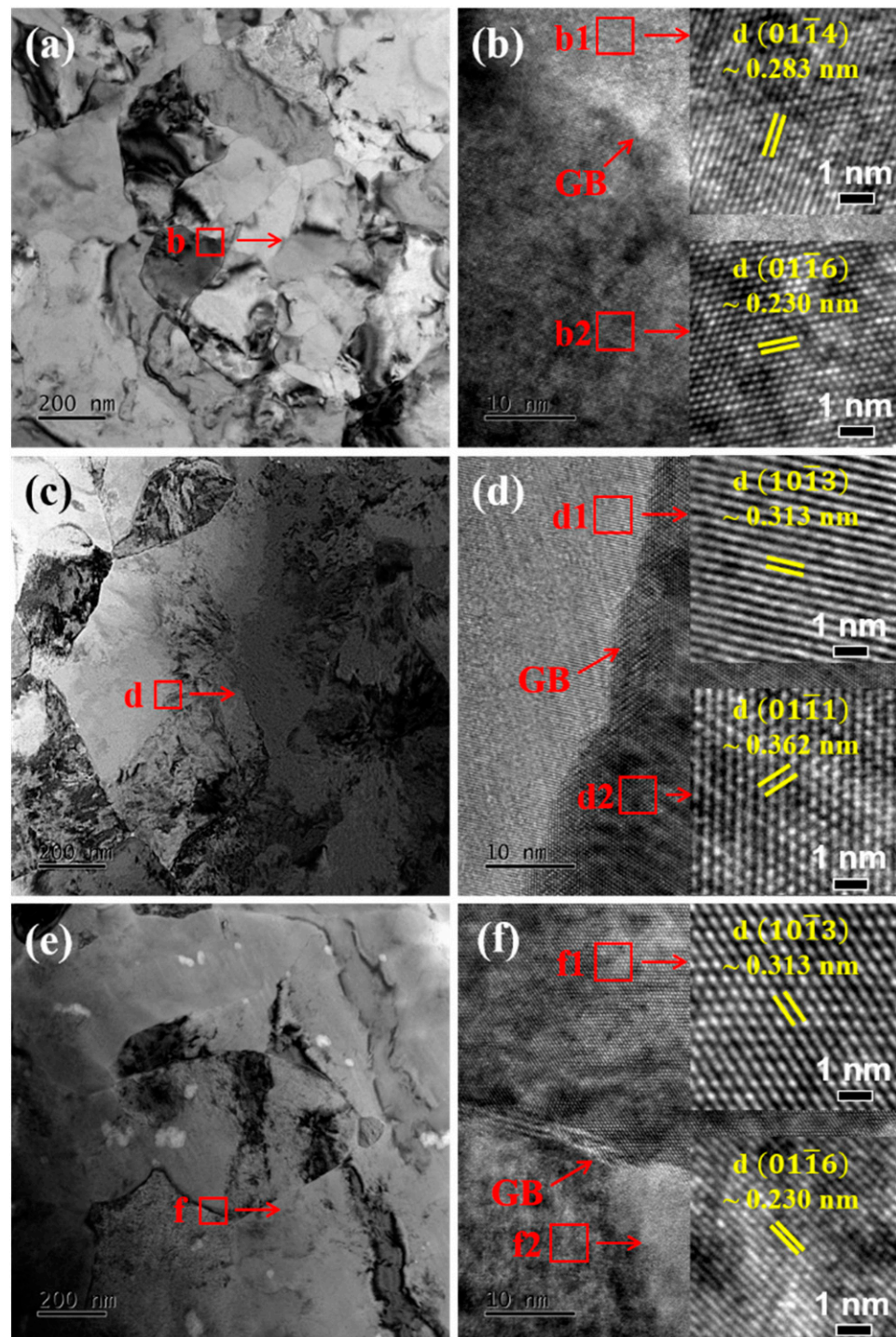


Figure 4. TEM bright-field (TEM-BF) images and high-resolution phase contrast (HRTEM) images near grain boundaries (GBs) of Sb_2Te thin films annealed at different temperatures: (a,b) 140 °C; (c,d) 200 °C; (e,f) 400 °C. The insets are the inverse fast Fourier transform (IFFT) images of the lattices on both sides of the grain boundaries.

Surface energy and strain energy are essential factors driving orientation preference. The role of surface energy on the prismatic preference of Sb_2Te thin film is analyzed in this segment. Table 1 gives the interplanar spacings of $(10\bar{1}3)$, $(01\bar{1}6)$, $(11\bar{2}0)$, and $(10\bar{1}0)$ planes. For the sake of comparison, the (0001) crystal plane that exhibits the maximum interplanar spacing in Sb_2Te lattice is also provided. It knows that a larger interplanar spacing means a lower surface energy [19]. Therefore, the surface energy of these crystal planes is arranged as follows: $(10\bar{1}0) > (01\bar{1}6) > (11\bar{2}0) > (10\bar{1}3) > (0001)$. It has been suggested that the minimum surface energy supports (0001) orientation formation in Sb_2Te thin film [20]. This implies that the surface energy is not the most important reason for prismatic preference.

Table 1. Interplanar spacings of $(10\bar{1}3)$, $(01\bar{1}6)$, $(11\bar{2}0)$, $(10\bar{1}0)$, and (0001) planes of Sb_2Te , data from reference [21].

Crystal Plane	$(10\bar{1}3)$	$(01\bar{1}6)$	$(11\bar{2}0)$	$(10\bar{1}0)$	(0001)
Interplanar Spacing (nm)	0.3131	0.2301	0.2360	0.1233	1.7633

Now we turn to the discussion of the contribution of lattice strain. The as-deposited Sb_2Te thin film is in amorphous state, which has disordered atoms with a lower density, whereas annealed Sb_2Te thin film is in crystalline state, in which the atoms are arranged in order. Accordingly, crystalline Sb_2Te thin film has a larger atomic density and a lower volume. The rearrangement of atoms could lead to strong volume contraction in the process of crystallization. Namely, disordered–ordered phase transition results in an increase in film density, accompanied by the decreased volume. The lattice strain that is induced by volume shrinkage after crystallization is regarded as an elemental origin. The density difference results from the distinct amorphous and crystalline atomic arrangements. Consequently, a thicker Sb_2Te film with a higher mass exhibits more pronounced volume shrinkage, which would promote a stronger lattice strain and prismatic preference. Therefore, we designed the thin film with two thicknesses (~ 200 nm and ~ 1000 nm) to demonstrate the contribution of the strain for the prismatic texture, and we speculated that the 1000 nm Sb_2Te thin film should exhibit a stronger $\{11\bar{2}0\}$ and $\{10\bar{1}0\}$ prismatic texture. Annealing temperature and annealing time affect the crystallization of PCM thin film. Previous results show that the crystallization temperature of Sb_2Te thin film is around 140°C . We employed the annealing processes (170°C : 10 min, 170°C : 15 min, 170°C : 25 min, and 170°C : 35 min) to reduce the effect of crystallinity on the diffraction intensity in XRD.

Figure 5 shows XRD patterns of 200 nm and 1000 nm Sb_2Te thin films annealed at 10 min, 15 min, 25 min, and 35 min. We focus on the strong $\{11\bar{2}0\}$ diffraction peak that is located at $\sim 42.2^\circ$. In 200 nm Sb_2Te thin film, the peak intensities of $\{11\bar{2}0\}$ planes are 3038, 6603, 6667, and 6353 when annealed at 10 min, 15 min, 25 min, and 35 min, respectively (Figure 5a). It also occurs in 1000 nm Sb_2Te thin film, in which the peak intensities are 15,922, 30,646, 30,708, and 30,895, respectively (Figure 5b). This indicates that Sb_2Te thin film annealed at 10 min is partially crystallized. After annealing at 15 min, both samples are fully crystallized. Figure 6 shows XRD patterns of 200 nm and 1000 nm Sb_2Te thin films annealed at 15 min and 35 min. All Sb_2Te thin films exhibit four narrow diffraction peaks. Diffraction peaks emerge at $\sim 28.7^\circ$, $\sim 39.8^\circ$, $\sim 42.2^\circ$, and $\sim 76.9^\circ$, corresponding to $\{10\bar{1}3\}$, $\{01\bar{1}6\}$, $\{11\bar{2}0\}$, and $\{30\bar{3}0\}$ planes. Table 2 gives the diffraction peak intensities. The peak intensities of the $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ diffraction planes in the 1000 nm Sb_2Te thin film are clearly higher than those in the 200 nm thin film. It implies that 1000 nm Sb_2Te thin film has a stronger $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ preference. More importantly, the $\{10\bar{1}3\}$ and $\{01\bar{1}6\}$ peak intensities of the two films are a little different. It means that the number of crystals involved in diffraction has a relatively weak effect on peak intensity. That is to say, the impact of film thickness on the diffraction strength is weak in the present result. Therefore, the degree of prismatic preference in 200 nm and 1000 nm Sb_2Te thin films could be discussed by using reasonable annealing processes (170°C : 15 min and 170°C : 35 min).

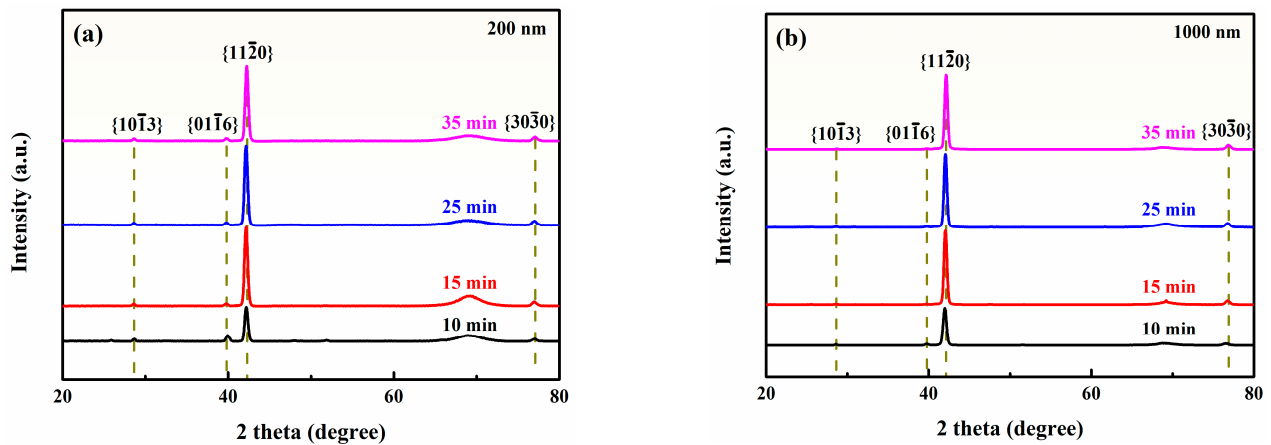


Figure 5. XRD patterns of 200 nm (a) and 1000 nm (b) Sb_2Te thin films annealed at different times: 10 min; 15 min; 25 min; 35 min.

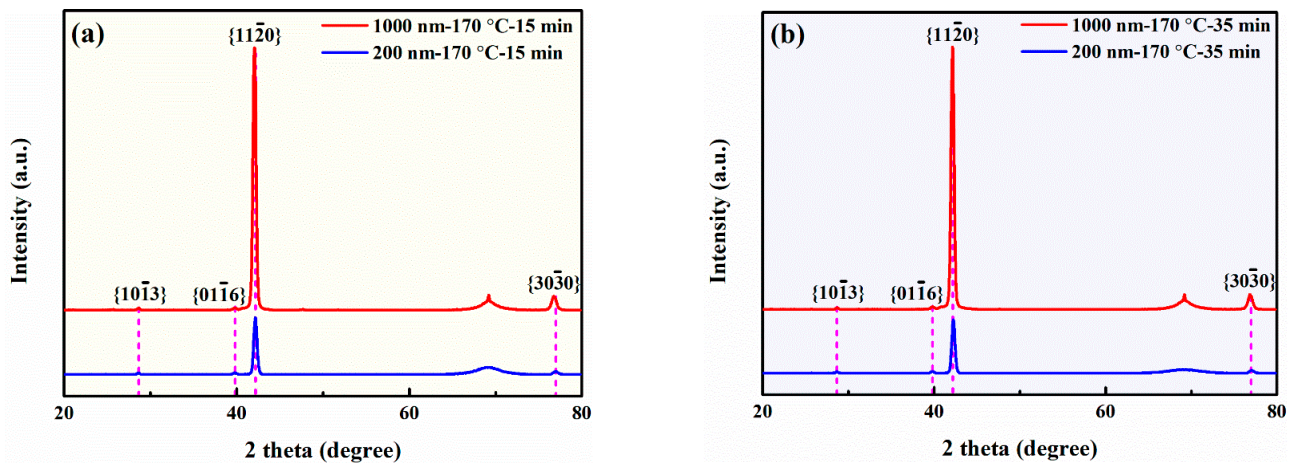


Figure 6. XRD patterns of 200 nm and 1000 nm Sb_2Te thin films annealed at different times: (a) 15 min; (b) 35 min.

Table 2. Diffraction intensities of $\{11\bar{2}0\}$, $\{30\bar{3}0\}$, $\{10\bar{1}3\}$, and $\{01\bar{1}6\}$ planes of 200 nm and 1000 nm Sb_2Te thin films annealed at 15 min and 35 min (shown in parentheses).

Annealing Time		15 min (35 min)			
Diffraction plane		$\{11\bar{2}0\}$	$\{30\bar{3}0\}$	$\{10\bar{1}3\}$	$\{01\bar{1}6\}$
Diffraction intensity (1000 nm)		30,646 (30,895)	1653 (1794)	233 (205)	257 (332)
Diffraction intensity (200 nm)		6603 (6353)	367 (357)	159 (173)	183 (198)

Figure 7 shows the measured $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ PFs of 200 nm and 1000 nm Sb_2Te thin films annealed at 15 min and 35 min. As displayed in the top panel, after annealing for 15 min, the maximum intensity of $\{11\bar{2}0\}$ PF is 9.02 for 1000 nm Sb_2Te thin film, higher than that in 200 nm Sb_2Te thin film (6.33). Simultaneously, in the 1000 nm Sb_2Te thin film, the maximum intensity of $\{30\bar{3}0\}$ PF is 6.20, which is twice that of the 200 nm Sb_2Te thin film (3.10). Moreover, maximum densities of $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ PFs are not significantly affected by the prolonged annealing time, as illustrated in the bottom panel. Therefore, 1000 nm (thicker) Sb_2Te thin film exhibits a stronger prismatic texture, consistent with XRD patterns and our predictions.

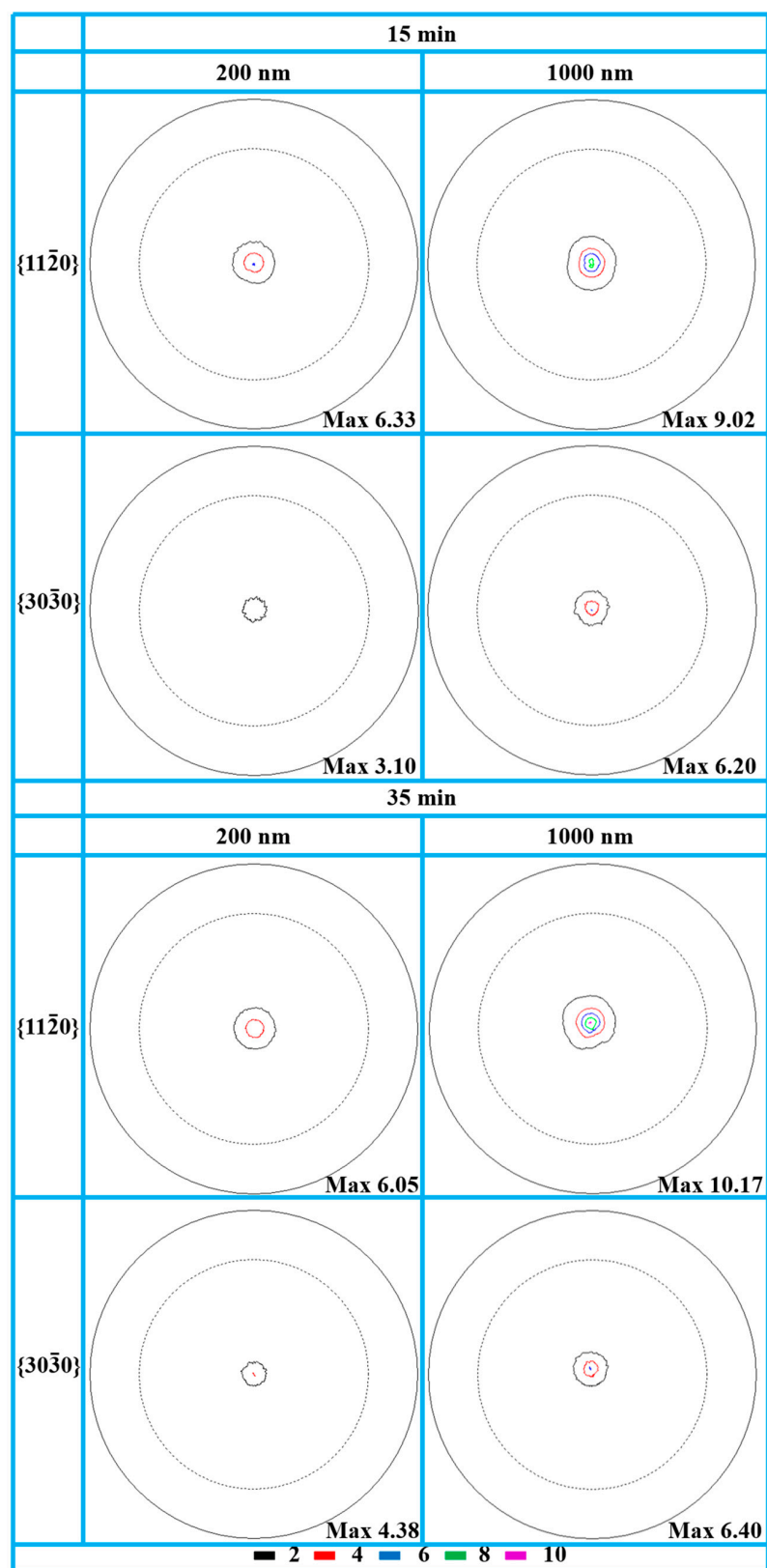


Figure 7. Measured $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ PFs of 200 nm and 1000 nm Sb_2Te thin films annealed at 15 min (**top** panel) and 35 min (**bottom** panel). Different colors represent pole density levels: black for 2, red for 4, blue for 6, green for 8, and lavender for 10. The maximum pole density is near the center of the measured PFs.

Mitra et al. [22] reported that the strain caused by the density difference between crystalline and amorphous states leads to the structural variations of the amorphous phase. It means that the minimization of the strain energy may provide driving force to deform the lattice. Mechanical analysis of a Sb_2Te unit cell offers insight into the strain-driven prismatic texture formation. The anisotropic modulus quantitatively describes the deformation resistance in various crystallographic orientation. Unfortunately, to the best of our knowledge, no experimental information on the anisotropic modulus of the Sb_2Te crystal was available to discuss. The anisotropic modulus originates from the bonding strength in different directions in the lattice. The stronger the bonding in a certain orientation, the greater the anisotropic modulus. The space group of Sb_2Te is $P-3m1$. The Sb_2Te lattice comprises octahedral Sb_2Te_3 and Sb_2Sb_2 structural primitives, which are stacked layer by layer along the c -axis. The atomic layers are bonded by van der Waals (vdW) bonds. Therefore, bonds in the prismatic orientation are weaker than in others, leading to a stronger tendency to deform. As found by Raoux et al. [23], the Sb_2Te lattice expands along the $\langle 0001 \rangle$ axis with the increased annealing temperature. It implies that the prismatic direction more easily deforms. Figure 8 shows the schematic diagram of Sb_2Te lattice, where the weak van der Waals bonds are located between the Sb–Sb and Sb–Te atomic layers.

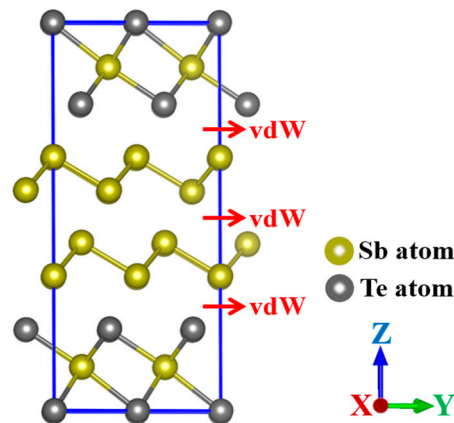


Figure 8. Schematic diagram of Sb_2Te lattice. The space group of Sb_2Te is $P-3m1$. There are van der Waals bonds along the c -axis. Sb atom is colored by brown and Te atom is marked by grey.

Table 3 gives the structural parameters of 200 nm and 1000 nm Sb_2Te thin films. After annealing for 15 min, the diffraction angles of $\{11\bar{2}0\}$ ($2\theta = 42.054^\circ$) and $\{30\bar{3}0\}$ ($2\theta = 76.757^\circ$) in the 1000 nm Sb_2Te thin film are lower than those in the 200 nm Sb_2Te thin film (42.170° for $\{11\bar{2}0\}$ and 77.010° for $\{30\bar{3}0\}$). Consequently, a larger lattice parameter (a) is shown for 1000 nm Sb_2Te thin film. Similar results are displayed for Sb_2Te thin film annealed at 35 min. The value of (a) measured by using power XRD is 0.4272 nm for single-crystal Sb_2Te [21], which is relatively close to the value of 200 nm Sb_2Te thin film (~ 0.4280 nm) and is clearly smaller than that of 1000 nm Sb_2Te thin film (~ 0.4290 nm). This could also infer that the degree of lattice distortion is higher in the 1000 nm Sb_2Te thin film. The lattice parameter (c) was not calculated because the diffraction signals of $\{10\bar{1}3\}$ and $\{01\bar{1}6\}$ planes are weak. In 1000 nm Sb_2Te thin film, a stronger volume shrinkage in the crystallization process induces a greater lattice strain. The c -axis with weaker bonding appears to be compressed. The a -axis is extended to maintain the stability of Sb_2Te lattice. Consequently, the 1000 nm Sb_2Te thin film exhibits a larger lattice parameter (a). This may be an acceptable explanation. Zhou et al. [20] suggested that Sb_2Te lattice with compressed c -axis is more stable because of the restricted atom free space. Therefore, the lattice strain is an important factor for the prismatic preference, and the prismatic texture could be maintained in Sb_2Te thin film. Note that differing surface energy may be the reason for the difference in the strength of $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ orientation. In addition, Sb_2Te thin film has coarser grains due to the grain-growth-dominated crystallization, which is not conducive to freeing the stress. Therefore, the prismatic texture of single-phase Sb_2Te thin

film is caused by the lattice strain, surface energy of the crystal plane, and coarse grain, where the lattice strain is a major contributor.

Table 3. Structural parameters (diffraction angle (2θ) and interplanar spacing (d) of $\{11\bar{2}0\}$ and $\{30\bar{3}0\}$ planes and lattice parameter (a) of 200 nm and 1000 nm Sb_2Te thin films annealed at 15 min and 35 min (shown in parentheses).

Sb ₂ Te Thin Film	{11 $\bar{2}$ 0}			{30 $\bar{3}$ 0}		
	2θ (°)	d (nm)	a (nm)	2θ (°)	d (nm)	a (nm)
200 nm	42.170 (42.232)	0.2141 (0.2138)	0.4282 (0.4276)	77.010 (77.078)	0.1237 (0.1236)	0.4286 (0.4283)
1000 nm	42.054 (42.150)	0.2147 (0.2142)	0.4294 (0.4284)	76.757 (76.854)	0.1241 (0.1239)	0.4298 (0.4294)

3.3. Electrical Properties of Prismatic Textured Sb_2Te Thin Film

We investigated the electrical properties of prismatic textured Sb_2Te thin film by using PPMS. Sb_2Te thin film exhibits p -type conductivity, which is consistent with other Sb-rich PCM thin films [24,25]. It suggests that the excited holes dominate the electrical transport in Sb_2Te thin film, originating from the structural vacancies. In Sb–Te binary alloys, Sb vacancies and Sb_{Te} antisite defects are confirmed to be the essential carriers [26]. Figure 9a shows the carrier mobility of as-deposited (amorphous) and annealed (crystalline) Sb_2Te thin films. Carrier mobility of as-deposited Sb_2Te thin film is $0.241 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, almost equal to the result ($0.220 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) [27]. In amorphous thin film, carrier mobility strongly depends on the localized state, which is related to the degree of structural disorder [28]. When the annealing temperature is 140°C , carrier mobility is maintained, which results from the weak crystallinity, as shown in XRD and EBSD. Therefore, carrier mobility may be susceptible to the atomic arrangement. In fully crystallized Sb_2Te thin film, carrier exhibits a higher mobility. We compared the carrier mobility of 200°C annealed Sb_2Te thin films with prismatic texture and with random orientation. It is obvious that textured Sb_2Te thin films have higher carrier mobility, as displayed in Figure 9a. We have reasons to suppose that prismatic texture promotes carrier migration. Texture formation improves the alignment and connectivity of grains in the thin film, which helps to increase the average free path of the carrier [29]. PCM thin film with fiber texture possesses more coincidence boundaries [30]. Grain boundary potential barrier is related to the misorientation of grains. As measured by Tsurekawa et al. [31], the potential barrier height of coincidence boundaries is lower than twice that of random boundaries. Therefore, in prismatic orientated Sb_2Te thin film, the carrier could encounter less grain scattering and trapping. It thus increases the mean free path and mobility of the carrier. As shown in Figure 9a, Sb_2Te thin film annealed at 400°C exhibits a stronger prismatic texture and carrier mobility. The impact of grain growth on the carrier transport should not be overlooked. It is stressed that grain with preferred orientation has greater growth advantage, which further reduces the grain boundary scattering effect. Therefore, there are two points in addressing the role of prismatic texture on carrier mobility in Sb_2Te thin film. On the one hand, prismatic texture improves the degree of atomic ordering and decreases the grain boundary potential barrier to enhance carrier transfer. On the other hand, grain with prismatic preferred orientation is further coarsened to facilitate carrier mobility.

Figure 9b shows the carrier density of as-deposited and annealed Sb_2Te thin films with prismatic texture. At higher annealing temperature (400°C), Sb_2Te thin film exhibits lower carrier density ($3.939 \times 10^{20} \text{ cm}^{-3}$) than that annealed at 200°C ($4.415 \times 10^{20} \text{ cm}^{-3}$). It implies that the vacancy density decreases at higher temperature. To our knowledge, texture formation may reduce the structural defects at the grain boundary. Nevertheless, dependence of carrier density on the texture needs to be addressed. From the viewpoint of carrier mobility, reducing the intensity of prismatic texture could inhibit carrier transport, thus improving the resistance of Sb_2Te thin film to decline power consumption.

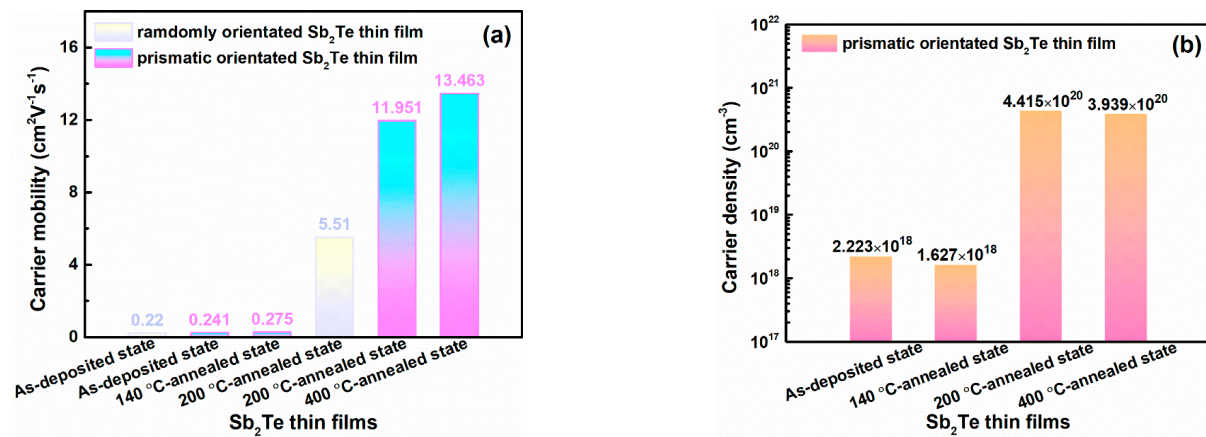


Figure 9. (a) Carrier mobility of as-deposited and annealed Sb₂Te thin films (200 nm) with prismatic texture and random orientation. Data of as-deposited and 200 °C annealed Sb₂Te thin films with random orientation from reference [27]. (b) Carrier density of as-deposited and annealed Sb₂Te thin films (200 nm) with prismatic texture.

3.4. Interface Stability of Prismatic Orientated Sb₂Te Thin Film

The formation of the texture alters the mismatch between the film and the substrate. It ultimately affects the stability of the film–substrate interface. Table 4 gives the calculated mismatches between the various crystal planes of Sb₂Te and Si (100) plane. The E2EM model [14,15] was used, where the crystal structure parameters of Sb₂Te and Si are obtained from references [21,32]. The calculation results show that the mismatches of (11 $\bar{2}$ 0)_{Sb₂Te} // (100)_{Si} and (30 $\bar{3}$ 0)_{Sb₂Te} // (100)_{Si} are higher than other matchings. In addition, prismatic orientated Sb₂Te exhibits higher mismatches with Si (110) and Si (111) planes, as given in Tables 5 and 6. Mismatch increases the interface energy, which may be the root of defect generation and element separation. It indicates that the formation of the prismatic texture may be unfavorable for the endurance of Sb₂Te thin film.

Table 4. Mismatch between the various crystal planes ((0001), (10 $\bar{1}$ 3), (01 $\bar{1}$ 6), (11 $\bar{2}$ 0), and (30 $\bar{3}$ 0)) of Sb₂Te thin film and the (100) crystal plane of Si substrate.

Matching Relation	(0001) _{Sb₂Te} //(100) _{Si}	(10 $\bar{1}$ 3) _{Sb₂Te} //(100) _{Si}	(01 $\bar{1}$ 6) _{Sb₂Te} //(100) _{Si}	(11 $\bar{2}$ 0) _{Sb₂Te} //(100) _{Si}	(30 $\bar{3}$ 0) _{Sb₂Te} //(100) _{Si}
Mismatch	0.624	1.119	1.884	2.107	4.381

Table 5. Mismatch between the various crystal planes ((0001), (10 $\bar{1}$ 3), (01 $\bar{1}$ 6), (11 $\bar{2}$ 0), and (30 $\bar{3}$ 0)) of Sb₂Te thin film and the (110) crystal plane of Si substrate.

Matching Relation	(0001) _{Sb₂Te} //(110) _{Si}	(10 $\bar{1}$ 3) _{Sb₂Te} //(110) _{Si}	(01 $\bar{1}$ 6) _{Sb₂Te} //(110) _{Si}	(11 $\bar{2}$ 0) _{Sb₂Te} //(110) _{Si}	(30 $\bar{3}$ 0) _{Sb₂Te} //(110) _{Si}
Mismatch	0.734	0.499	1.039	1.197	2.805

Table 6. Mismatch between the various crystal planes ((0001), (10 $\bar{1}$ 3), (01 $\bar{1}$ 6), (11 $\bar{2}$ 0), and (30 $\bar{3}$ 0)) of Sb₂Te thin film and the (111) crystal plane of Si substrate.

Matching Relation	(0001) _{Sb₂Te} //(111) _{Si}	(10 $\bar{1}$ 3) _{Sb₂Te} //(111) _{Si}	(01 $\bar{1}$ 6) _{Sb₂Te} //(111) _{Si}	(11 $\bar{2}$ 0) _{Sb₂Te} //(111) _{Si}	(30 $\bar{3}$ 0) _{Sb₂Te} //(111) _{Si}
Mismatch	0.783	0.224	0.665	0.794	2.107

In order to achieve low power consumption and high endurance of PCM device, we suggest reducing the density of prismatic texture in Sb₂Te thin film. Lattice strain has been found to be a major contributor of prismatic preference in Sb₂Te thin film. Strain

resistance of Sb_2Te lattice could be improved by introducing strong chemical bonds, which helps reduce the intensity of prismatic texture. Increased deformation resistance means that Sb_2Te thin film has better mechanical properties. Moreover, strengthening chemical bonds would improve the structural rigidity. It is favorable for a longer data retention. Therefore, chemical bonding modification may be a selective method to tune the texture and properties of Sb_2Te thin film. Decreased prismatic texture density means that Sb_2Te thin film has a random orientation or other sharp texture components. It is reported that basal textured PCM thin films exhibit improved switching properties [8,33–35], making orientation optimization of PCM thin film valuable.

4. Conclusions

The texture of Sb_2Te thin films with different thicknesses annealed at various temperatures and times is investigated. The formation mechanism of prismatic texture is revealed. Electrical properties and interfacial stability of prismatic-preferred Sb_2Te thin film are analyzed. This work is expected to provide references for controlling texture features and improving properties of PCM thin films. The following conclusions can be drawn from this work:

1. The single-phase Sb_2Te thin films exhibit $\{11\bar{2}0\}$ and $\{10\bar{1}0\}$ prismatic texture.
2. The $\{11\bar{2}0\}$ and $\{10\bar{1}0\}$ prismatic preference is induced by the lattice strain, surface energy of the crystal plane, and coarse grain, where the lattice strain is a major contributor.
3. The prismatic-preferred Sb_2Te thin film exhibits higher carrier mobility compared with its randomly orientated counterparts. The increase of carrier mobility results from the reduction of grain boundary potential energy and grain coarsening in the prismatic-textured Sb_2Te thin film.
4. The prismatic-preferred Sb_2Te thin films have higher mismatches with (100), (110), and (111) oriented silicon wafers, which reduces the stability of the thin film–substrate interface.

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