Superlattice-like Structure Phase Change Materials for Data Storage

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ABSTRACT

Phase change materials are critical for data storage applications. However, suitable phase change materials are limited by nature due to the constraints of their contradictory properties. To overcome these problems, one possible approach is to make phase change materials with artificial structure such as superlattice-like (SLL) structure. A properly designed SLL structure could balance the properties of the component materials, e.g. the phase change speed and stability. In this work, the application of SLL phase change structures on data storage, e.g. optical rewritable disk and PCRAM are introduced. The SLL optical disc possesses a better recording property compared to conventional disc. The effect of the anisotropic thermal conductivity of SLL phase change layers on the thermal profile of PCRAM devices with conventional structure and line-type structure is investigated by simulation. The simulation results show that the effect is device geometry dependent. Proper control of the SLL PCRAM structure and thus its anisotropic thermal conductivity along in-plane and cross-plane would allow the thermal management of the devices based on different application requirements.

Key words: Optical disc, PCRAM, superlattice, phase change materials

1. INTRODUCTION

Chalcogenide-based phase change materials have been found to be useful for many applications, which include optical disc, electrical switches, memory technologies, and potentially many others that can utilize its unique phase change property. Among the most important applications are optical rewritable disc and phase change random access memory (PCRAM) [1-3]. In optical rewritable disc, laser pulses cause the switching of phase change materials between amorphous and crystalline states. The reflectivities for the two states are different and detected for data storage application. In PCRAM, the switches between the high resistance amorphous and low resistance crystalline states are induced by electrical pulses and the different resistance is detected. Among the chalcogenide-based phase change materials, GeSbTe system is the most widely applied phase change alloy for both optical rewritable disc and PCRAM devices.

Although ongoing research and development have proven the great potentials of phase change materials, there are still several issues concerning their applications. One of them is the crystallization speed of the material, which has yet to be improved to a level to match the requirements of applications. Another more general issue is the challenging request for phase change materials that can meet the requirements of a particular application, as all the desired properties are usually not found in a single material. However, the suitable phase change materials for these applications are limited due to the limited phase change materials available in the nature and the constraints by the contradictory phase change properties requested by applications, such as speed and stability. Hence, it is very important to explore new phase change materials.

One possible approach is to make phase change materials with artificial structures. A superlattice-like (SLL) structure for phase change materials has recently been studied and is in active development. The basic concept is to alternatively deposit two phase change materials, one with a high crystallization speed while the other with a relatively low crystallization speed but a high stability, to form the SLL structure. It has been found that a properly designed SLL structure could balance the properties of the component materials, for example, the phase change speed and stability [4-6].

In this work, the application of SLL phase change structures on data storage, e.g. optical rewritable disc and PCRAM are introduced by both simulation and experiments.

2. SLL CONCEPT AND THEORETICAL CONSIDERATION

There are several considerations for using the SLL structure in data storage e.g. optical rewritable disc and PCRAM. In terms of crystallization and thermal conductivity considerations, SLL structures are better as compared to the conventional bulk-layer structure.

Material considerations: For the application in PCRAMs, phase change materials must have many desirable properties, e.g. high speed and thermal stability. However, it is difficult to find phase change materials, e.g. GeSbTe alloy that can fulfill all the requirements. In SLL structures, properties such as melting and crystallization temperatures can be controlled by the configurations of the SLL layers.

Thermal considerations: Density, specific heat and thermal conductivity are the basic parameters for the thermal profiles. The density of crystalline state is smaller than that of amorphous state but with slight difference. Both amorphous and crystalline structures of the same material can be expected to have the same or similar specific heat value if it mainly related to the vibration modes that are corresponding closely to those of a fully excited harmonic oscillator. Hence, the contribution of density and specific heat between bulk and SLL materials is not critical. However, significant reductions in both the in-plane and cross-plane thermal conductivities of superlattices have been observed experimentally. Theoretical studies have revealed that the thermal conductivities along both in-plane and cross-plane directions deviate significantly from its constituent bulk materials. The thermal conductivity of SLL is much reduced compared to the bulk. The reduction is mainly attributed to the interfaces and phonon scattering within the superlattice.

Crystallization considerations: According to the classical crystallization theory, the crystallization of bulk materials is a nucleation followed by a subsequent growth. SLL structure can enhance the crystallization of the phase change materials. The fast crystallization material will crystalline first and then acts as an induced layer for the slow crystallization material to enhance nucleation and rapid crystal growth. In SLL the crystallization, e.g. crystallization temperature, is related to the thickness of the elemental layer and also related to the capping layer materials. By controlling the SLL structure properly, the crystallization temperature can be designed based on the requirement of the devices.

Electrical considerations: The electrical properties of superlattice structures have been widely studied in the last few decades. They are found to be dependent on the superlattice periods and thickness of the incorporated materials. In the application on optical disc, there is no electron movement for the light induced phase change. However, in PCRAM, there is electron movement cross the device for the electric induced phase change. The scattering of electrons at the boundary and interfaces will significantly affect the performance of the device.

3. APPLICATION OF SLL PHASE CHANGE STRUCTURE ON DATA STORAGE
3.1 SLL OPTICAL REWRITABLE DISC

In this work, the SLL disc incorporating $GeTe/Sb_2Te_3$ and conventional disc with $Ge_1Sb_2Te_4$ and $Ge_1Sb_4Te_7$ were studied by simulation using in-house developed simulation software. The mark shapes were simulated at different speed by considering the reduction of the thermal conductivity of the SLL structure.

In the simulations the thermal properties of the materials are assumed to be independent of temperature. It is also assumed that the electrical properties of the materials in the structure are isotropic homogeneous and independent of temperature. Latent heat is not considered because it is much smaller than that of Joule heating.

The thermal transfer process obeys the standard heat transport equation:

$$\nabla \cdot k\nabla T + Q = \rho \frac{\partial T}{\partial t} \qquad (1)$$

where, ∇ is the gradient operator, t is the time, T is the temperature, c is the specific heat, k is the thermal conductivity, ρ is the density, and Q is the Joule heat per unit volume and per unit time, which is called heat density. It can be further simplified into a static magnetic analysis since the voltage applied to the electrodes remained unchanged. In the static field analysis, the Joule heating density distribution can be described as the following:

$$Q = \frac{1}{n}\sum_{i=1}^{n}[\sigma]\{J_i\}\{J_i\} \qquad (2)$$

where, n is the number of integration points, $[\sigma]$ is the resistivity matrix and $\{J_i\}$ is the total current density in the element at integration point i.

Fig. 1 shows the simulated mask shapes comparison between discs with SLL structure, $Ge_1Sb_2Te_4$, $Ge_1Sb_4Te_7$ at different rotation speed. It can be clearly seen that the mark shapes of the $Ge_1Sb_2Te_4$ and $Ge_1Sb_4Te_7$ disc couldn't be written well at speed of 10 m/s and 12 m/s. However, SLL disc demonstrates good simulated mark shapes at a rotation speed as high as 18 m/s, which shows the SLL disc possessing a much better recording property compared to $Ge_1Sb_2Te_4$ and $Ge_1Sb_4Te_7$ discs.

The simulation results have been confirmed by experiments. Fig.2. shows the experimental eye-patterns of (a) $Ge_1Sb_2Te_4$ disc 1×, 18.9 m/s, (b) $Ge_1Sb_2Te_4$ disc 10×, 18.9 m/s, (c) SLL disc 1×, 18.9 m/s, (d) SLL disc 10×, 18.9 m/s, respectively. For $Ge_1Sb_2Te_4$ disc, the 3T to 14T signals can be easily distinguished for one time writing at 18.9 m/s. However, the signals cannot be distinguished after ten times writing. In contrast, for SLL disc, the signals are still clear after ten times writing at 18.9 m/s. This reveals that, at higher rotation speeds, amorphous marks can be written and erased much more quickly for SLL disc, thus shortening the crystallization time and increasing the data transfer rate.

3.2 SLL PCRAM WITH CONVENTIONAL STRUCTURE

PCRAM is considered as one of the best candidates for the next-generation nonvolatile memory (NVM) due to its near-ideal NVM advantages. The SLL PCRAM has demonstrated both a high speed and a good stability [5]. It was found that the main reason for the excellent performances of SLL PCRAM is due to the much lower thermal conductivity of the SLL material compared to that of bulk materials. The thermal conductivity of SLL structure has been experimentally found to be reduced to smaller than 30% of bulk material. The reduction of thermal conductivity and its effect on PCRAM device has been investigated by simulation in the paper presented in E*PCOS2006 [6]. The results showed that higher maximum temperature could be obtained using SLL structure due to its lower thermal conductivity. In that paper, the thermal conductivity was treated as isotropic. However, due to different interfaces and phonon scattering, the SLL structure may display anisotropic thermal conductivity which is different in the in-plane and cross-plane directions. In this work, the thermal performances of the cell as a result of anisotropic homogeneous thermal conductivity of the phase change layer were quantified. In this simulation, the anisotropic thermal conductivity of SLL structure was varied in the range of 50% to 150% of the bulk materials along in-plane (refer as X - axis) and cross-plane (refer as Y - axis), respectively.

Fig. 3 is the schematic cross-section of the SLL PCRAM device structure. The simulation studies were carried out by applying electrical pulse with a constant voltage. The PCRAM structure simulated in this work has a cell radius of 45 nm. The structure is firstly applied with an electrical pulse of 1 V bias for 50 ns before cooling it for the next 50 ns. The temperature distribution, the achievable highest temperature, the temperature history and the heating and cooling rates were simulated and analyzed for different SLL structures, respectively.

Fig. 4 shows the cross-sectional views of the temperature distribution in the phase change layer with the thermal conductivity of (a) X=50%, Y=100%, (b) X=100%, Y=100%, (c) X=150%, Y=100%, (d) X=100%, Y=50%, and (e) X=100%, Y=150% of that of bulk material, respectively. It can be seen that both top and bottom electrodes are served as heat sink. The thermal distribution is highly dependent on the thermal conductivity of the phase change layers. The heat is mainly confined within the phase change layer when its thermal conductivity is small. However, with the thermal conductivity increasing, more heat spreads into the surrounding dielectric layers. As the thermal conductivity further increases, the heat starts to spread towards the bottom while more heat spreading for higher thermal conductivity along the cross-plane.

Fig. 5 shows the temperature history during the electrical pulse at the center point of the phase change layer with different thermal conductivity. It showed that higher temperature is obtained with lower thermal conductivity. The cross-plane thermal conductivity is more critical than that of the in-plane on the effect towards the temperature profile. The temperature profiles display a smaller variation for the structure with in-plane thermal conductivity adjustment while a much larger variation for that with cross-plane adjustment.

Fig. 6 plots the maximum temperature achieved for different thermal conductivity. It can be seen that the achieved maximum temperature is highly dependent on the thermal conductivity. When the thermal conductivity reduces from 150% to 50% of the bulk, the temperature of the structure is increased from 610°C, 506°C, 481°C to 735°C, 936°C and 1125°C for the in-plane, cross-plane and both-plane adjustment, respectively. It shows that the reduction of the cross-plane thermal conductivity could effectively increase the maximum temperature. These results indicate that the PCRAM cell with lower thermal conductivity requires less input power to program the device especially during RESET process. These results also suggest that the thermal performance of the SLL PCRAM can be controlled and modified by designing the SLL structure with different in-plane and cross-plane thermal conductivity.

The heating rate against different thermal conductivity along in-plane and cross-plane are plotted in Fig. 7 (a) and (b). It can be seen that smaller thermal conductivity induces higher heating. However higher heating rate is obtained with the reduced cross-plane thermal conductivity.

3.3 SLL LINE-TYPE PCRAM

Recently, an advanced line-type PCRAM structure has attracted great interests [7]. This line-type PCRAM has an ultra-thin line of phase change material surrounded by dielectric. An electric current is used to heat the material to its phase change temperature, where it switches reversibly between crystalline and amorphous phases. Because the thin phase change was surrounded by dielectric which has lower thermal conductivity, line-type PCRAM dissipates little power and current. In this work, the line-type SLL PCRAM and the effect of the thermal conductivity of the phase change layer on the devices are also investigated by simulations.

Fig. 8 shows the cross-sectional views of the temperature distribution in the phase change layer with the thermal conductivity of X=50%, Y=50% of that of bulk material. It can be seen that when the thermal conductivity is reduced, heat is almost confined within the phase change layer.

Fig. 9 shows the temperature history at the PC layer center with (a) isotropical change and (b) anisotropical change of the thermal conductivity for line-type SLL PCRAM. Same as the conventional SLL PCRAM, when the thermal conductivity is isotropically reduced the device will achieve higher temperature. However, the behavior of the anisotropically changed thermal conductivity on line-type SLL PCRAM is different from that on conventional SLL PCRAM. It can be seen from Fig. 9 (b) that the change of the cross-plane thermal conductivity shows much more effect on the temperature while that of the in-plane has less effect. The results suggest that the effect of the anisotropic thermal conductivity on PCRAM is geometry dependent. Properly controlling the SLL structure and thus its anisotropic thermal conductivity along in-plane and cross-plane, the thermal profile of the devices can be designed based on the different requirement of the devices.

4. CONCLUSION

In this paper, the SLL structure phase change materials and its applications on data storage, e.g. optical rewritable disk, PCRAM, line-type PCRAM have been discussed. The thermal simulation and analysis on both conventional PCRAM and lone-type PCRAM with SLL structure were conducted by considering the variation of the anisotropic thermal conductivity of the phase change layer. The thermal performance, such as temperature profile, temperature history, heating and cooling rates and its dependence on the anisotropic thermal conductivity was simulated. The thermal performance of the SLL PCRAM was found to be highly dependent on the thermal conductivity. For the conventional SLL PCRAM devices, higher temperature is reached with the reduction of the thermal conductivity either isotropically or anisotropically. The cross-plane thermal conductivity is more critical than that of the in-plane on the effect towards the temperature profile. For the line-type SLL PCRAM, the cross-plane thermal conductivity shows much more effect on the temperature while that of the in-plane has less effect. The simulation results show that the effect of the anisotropic thermal conductivity on PCRAM is geometry dependent. Properly controlling the SLL PCRAM structure and thus its anisotropic thermal conductivity along in-plane and cross-plane, the thermal profile of the devices can be designed based on the different requirement of the devices.

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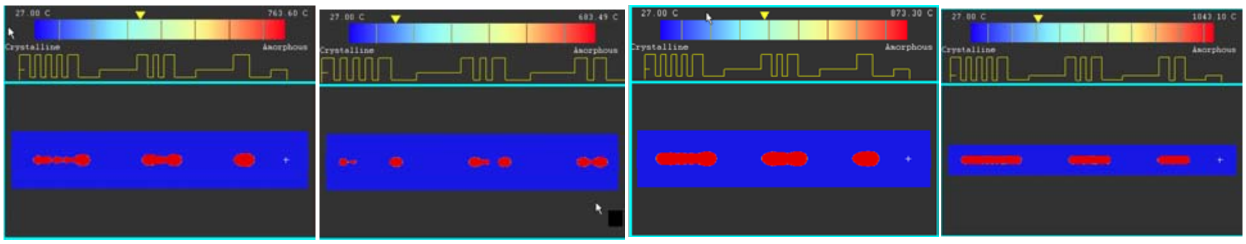
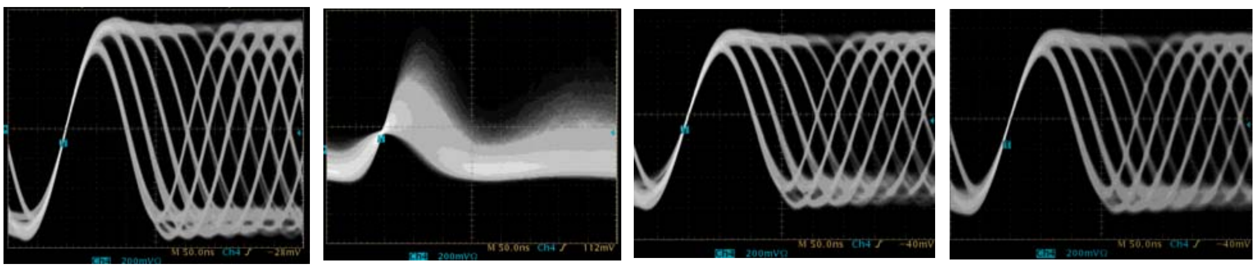
BIOGRAPHYICS

Zhao Rong received her Ph.D. degree in electrical and computer engineering from National University of Singapore in 1999. Her Ph.D. topic was application of low-temperature grown GaAs on quantum well laser on Si substrate using Molecular Beam Epitaxy growth. In 1998, she joined the Optical Media group in Data Storage Institute, Singapore, where she was involved in the development of high density re-writable optical disk. Since 2001 she has been working on the development of phase change random access memory (PCRAM). Currently she is a research scientist. Her current research activities include the device design, fabrication and characterization of PCRAM devices. Her research interests also include nano-fabrication using e-beam lithography and its application on data storage.



$Ge_1Sb_2Te_4$, v=10m/s $Ge_1Sb_4Te_7$, v=12m/s SLL, v=10m/s SLL, v=18m/s

Fig. 1 Mask shapes comparison between discs with SLL structure, $Ge_1Sb_2Te_4$, $Ge_1Sb_4Te_7$ at different rotation speed



(a) (b) (c) (d)

Fig. 2 The eye-patterns of (a) $Ge_1Sb_2Te_4$ disc 1×, 18.9 m/s, (b) $Ge_1Sb_2Te_4$ disc 10×, 18.9 m/s, (c) SLL disc 1×, 18.9 m/s, (d) SLL disc 10×, 18.9 m/s.

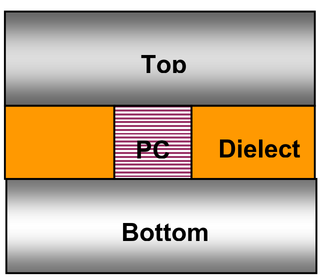
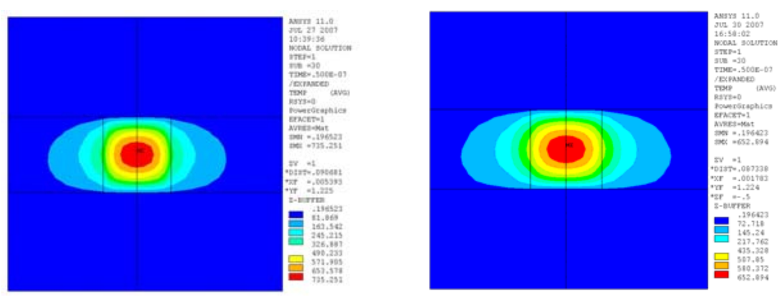
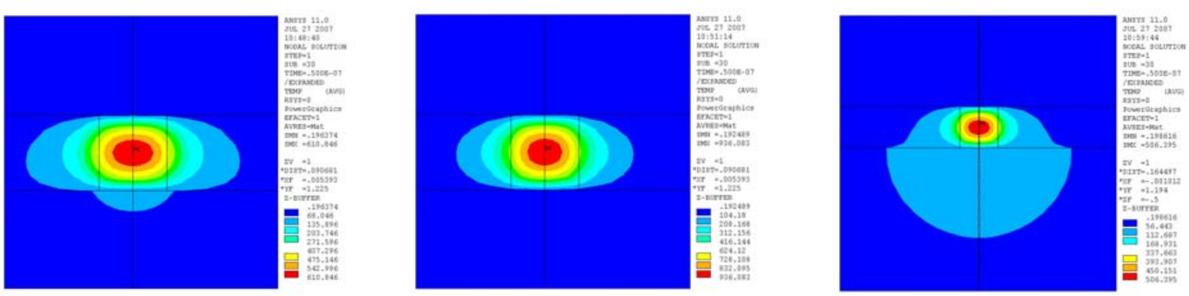


Fig. 3 Cross-section of SLL PCRAM

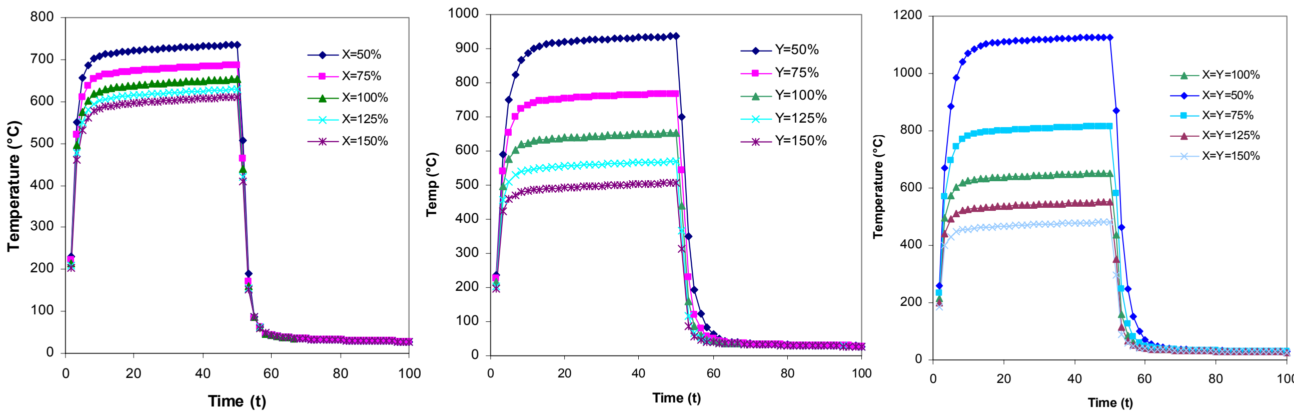


(a) (b)



(c) (d) (e)

Fig. 4 The cross-sectional views of the temperature distribution in phase change layer with its thermal conductivity of (a) X=50%, Y=100%, (b) X=100%, Y=100%, (c) X=150%, Y=100%, (d) X=100%, Y=50% and (e) X=100%, Y=150% of that of bulk material, respectively for conventional SLL PCRAM.



(a) (b) (c)

Fig. 5 The temperature history at the phase change layer center with different thermal conductivity (a) in-plane, (b) cross-plane, and (c) both in-plane and cross-plane, repectively for conventional SLL PCRAM.

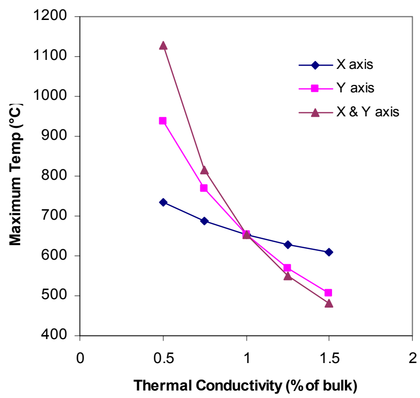
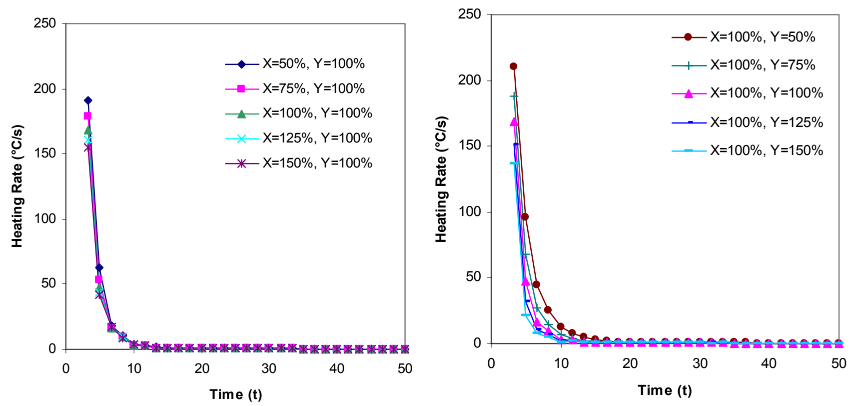


Fig. 6 The maximum temperature achieved for conventional SLL PCRAM with different thermal conductivity.



(a) (b)

Fig. 7 The heating rate for different thermal conductivity along (a) X-axis, and (b) Y-axis, respectively for conventional SLL PCRAM.

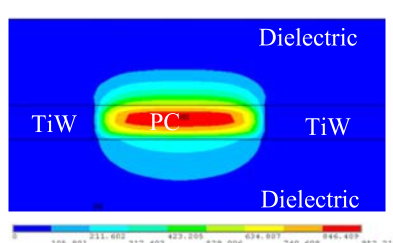


Fig. 8 The cross-sectional view of the temperature distribution in phase change layer with thermal conductivity X=50%, Y=50% of that of the bulk for line-type SLL PCRAM.

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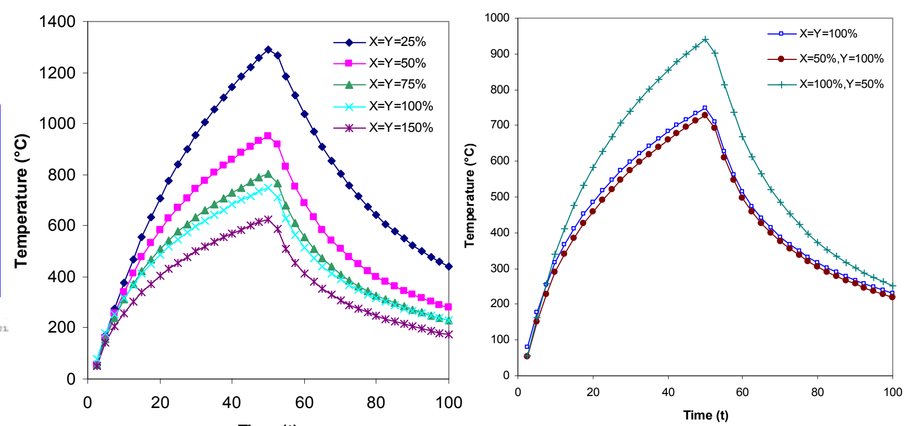

(b)

Fig. 9 The temperature history at the PC layer center with (a) isotropical change and (b) anisotropical change of the thermal conductivity for line-type SLL PCRAM.