Material Design of In₃SbTe₂ for Fast Switching Phase Change Memory

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Abstract

To develop low power consumption and fast switching phase change memory, a new phase change material has been designed with computational high-throughput method. Among several candidates, Y is chosen as an ideal dopant for In₃SbTe₂ (IST) phase change material and the Y doped IST PRAM cell devices show faster set/reset operation than undoped IST and GeSbTe due to fast phase changing mechanism at lower melting temperature.

1. Introduction

Phase-change random access memory (PRAM) has been investigated as an emerging non-volatile memory device. Recently, for the neuromorphic and 3D XPoint memory applications, fast switching speed, low power consumption, long retention, and excellent endurance are critical issues. Since the PRAM stores data with reversible phase change process between crystalline and amorphous state by Joule heating, the unstable phase changing temperature and switching speed are main drawbacks for achieving the 3D Xpoint memory and synaptic devices with low power consumption. The electrical performance of these devices are also strongly related with phase changing mechanism, which is dominantly controlled by lattice distortion and vacancy in the phase change materials. Thus far, many researchers have been tried to improve the properties of phase change materials by doping since doping element generates lattice distortion and vacancy, which will be key factor to design a novel phase change material [1]. From previous study [2, 3], In₃SbTe₂ (IST) phase-change material has multi-step phase transition temperatures and more stable than Ge₂Sb₂Te₅ (GST). However, the set/reset switching speed of the IST PRAM is slower than that of GST devices.

In this work, we have investigated to improve the properties of IST by doping several candidate elements. The idea is based on the lattice distortion led to faster operation speed and lower melting temperature [4, 5]. To find the ideal dopant that maximizes the effect of the lattice distortion, we have suggested two criteria; i) the enthalpy changes and ii) distortion angles at each doping site, which are carefully investigated through computational high-throughput screening method using density functional theory (DFT) and Ab initio molecular dynamics (AIMD) simulation as well as atomic structure analysis with high resolution transmission microscopy.

2. Experiments

The IST and doped IST thin films are co-sputtered with In₃SbTe₂ and dopant targets. The 15 dopant elements are selected from previous reports [1, 3] and the composition of sputtered doped IST is X12~13(In3SbTe2)88~87 (X is doping element). The IST and GST are sputtered by single targets of In₃SbTe₂ and Ge₂Sb₂Te₅, respectively. The sputtering process are conducted at room temperature in an Ar atmosphere. The PCRAM devices are fabricated with cell size of 250 nm x 250nm. HRTEM analysis was conducted using FEI TITAN at 300kV. DFT calculations are performed with the Vienna ab initio simulation package (VASP) program using the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) parameterization. In these DFT calculations, Kohn-Sham orbitals are expanded with a cut-off energy of 400.0 eV, and a 2×2×2 equally spaced k-point grids are used for the Brillouin zone sampling.

3. Results and discussion



Figure 1. A schematic high-throughput screening process for materials design using DFT and AIMD

Figure 1 shows the schematic diagram to design the novel phase-change materials. As it can be seen, many dopants, mainly used for semiconductor field, are calculated by computational high-throughput screening method using density function theory (DFT). The dopants are analysed with how large the distortion angle is made in the IST material with thermodynamically stable state ($E_{form} < 0$).

Dopant –	(a) Doping formation energy (eV/atom)			(b) Ionic radius dif-	(c) Distortion
	In-site	Sb-site	Te-site	ference (Å)	angle (degree)
Ag	2.42*	2.61	3.41	0.30	2.51
Bi	1.84	-0.36*	2.41	0.23	2.28
Er	0.20*	2.51	3.56	0.09	1.49
Ga	1.91*	2.33	3.24	-0.18	2.20
Gd	-0.8*	6.89	8.57	0.14	1.58
Ir	1.87*	3.59	3.95	-0.12	1.94
Ge	6.87*	7.22	8.00	-0.27	6.45
Та	3.38*	6.22	7.34	-0.08	7.36
Zr	1.2*	3.94	5.1	-0.08	12.4
Si	2.58*	2.97	3.66	-0.40	5.21
La	-0.15*	1.82	3.32	0.23	1.90
V	2.78*	4.82	6.95	-0.16	6.17
Y	-0.57*	2.10	3.01	0.10	2.00
Ti	1.98*	2.26	3.31	-0.13	4.37
Zn	2.36*	2.64	3.52	-0.06	2.99

Table 1. (a) Doping formation energy at each site (In, Sb, and Te) of selected elements, (b) the ionic radius difference between the dopant and the host ion, and (c) the distortion angle at the most stable site.

Table 1 shows the doping formation energy of each element substituted into In, Sb, and Te sites in the IST atomic structure. The energy indicates the stability of dopants when a dopant occupies a host site among In, Sb, and Te. If the energy is a negative value, the dopant is stable at the site. On the other hand, the positive value means that the dopant is unstable at the site and it can cause the phase separation while phase change is reversibly repeated during the set/reset operations. Only Y, Gd, Bi, and La elements have negative formation energy as indicated in Table 1. Among these four dopants, the Y seems to be the most proper dopant in the IST because the Y substitutes the In site with negative formation energy and the lattice angle is larger than the angles of the others. The distortion is definitely related with vacancy concentration and low activation energy for phase transition.



Figure 2. HRTEM images of Y-IST thin film. XRD spectra of the Y-IST thin film after the annealing at 450°C.

HRTEM images (Fig. 2) of the Y-IST thin films show the real atomic structure as the evidence of substitutional doping by Y atoms. The angular difference between the inter-planar angles of the IST and the distorted Y-IST is in the range from 0.25° to 1.98°, indicating that the maximum angular distortion ($\Delta \theta_{max}$) by the Y atom is 1.98°, which is well matched with 2.0° calculated by DFT. XRD pattern shows that the peaks of In and In₂O₃ are observed with the peak of the IST phase, but Y₂O₃ peak is not appeared. This means that the Y atoms substitute the In atom in the IST, forming the locally distorted Y-IST. Fabricated devices show that the Y doped IST (Y-IST) has fastest set/reset operations among Bi-IST, IST, GST PRAMs. AIMD simulation suggests that the transition time from crystalline to amorphous Y-IST is also faster than other materials due to the distorted lattice.



Figure 3. Electrical characteristics of (a) set (b) reset operations of the Y-IST, Bi-IST, IST, and GST PRAMs

4. Conclusions

A noble phase change material has been designed by computational high-throughput screening method. The calculated formation energy and lattice distortion angle in IST phasechange materials suggest an ideal dopant, in this work, Y for IST and real atomic structure of Y-IST is well matched with the theoretical prediction. The PRAM devices fabricated with Y-IST also shows fast set/reset operations and low power consumption during the set/reset operations. This result will be useful to design a new material for PRAM and neuromorphic synaptic devices.

5. Acknowledgements

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