JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS Vol. 13, No. 11-12, November – December 2011, p. 1594 - 1596

Influence of defects on the switching speed of $Ge_2Sb_2Te_5$

A. VELEA*, M. POPESCU, A. LÖRINCZI, F. SAVA, I. D. SIMANDAN, C. MIHAI[a]
National Institute R&D of Materials Physics, Bucharest-Măgurele, P. O. Box MG.7, Romania
[a]*Faculty of Physics, University of Bucharest, 405 Atomistilor str., P.O.Box MG-11, 077125, Măgurele-Ilfov, Romania*

Chalcogenide phase change materials are one of the major contenders for the new non-volatile memory applications. Here is reported that the switching speed of $Ge_2Sb_2Te_5$ is strongly dependent on the percent of defects in the material. Using cellular automata simulations it was shown that the size of the percolation cluster is minimum, thus the switching speed is maximum, for a percent of around 25% defects in the material. This is a property of the $Ge_2Sb_2Te_5$ that can be useful for new phase change materials and devices design with better switching properties.

(Received November 1, 2011; accepted November 23, 2011)

Keywords: Chalcogenide, Phase change materials, Cellular automata, Switching speed, Defects

1. Introduction

We are in the age of 'Big data' [1], datasets whose size is beyond the ability of typical database software tools to capture, store, manage, and analyze. Studies revealed that the total amount of data generated, stored, and consumed in the world in 2010 was about 13 exabytes. It is generated so much data today that it is physically impossible to store it all, so there is a need for higher capacity and more efficient storing devices.

Charge storage memories are reaching miniaturization limits because it becomes very difficult to hold enough electrons in those shrinking cells [2]. While magnetic and ferroelectric random access memories have problems with scalability, nonvolatile memories are increasingly investigated. Nonvolatile memories include phase-change memory in chalcogenides, programmable-metallization-cell memory in solid electrolytes, and resistance-change memory in transition-metal oxides. From those three classes the most significant is phase change memory.

Phase change materials were first studied by S. R. Ovshinsky [3]. These materials store data in a chalcogenide glass, using small voltage to switch sections of the material between two different states [4]. In one state, the atoms of the glass are arranged in an ordered crystal lattice, while in the other state they have an amorphous, disorganized arrangement. By applying a voltage across the electrodes, the entire material can be switched to any number of states along a continuum from totally unstructured to highly crystalline. The memory is read out by using another electrical pulse to measure the resistance of the material, which is much lower in the crystalline state.

Memory chips based on phase change materials perform faster than the flash memory chips when it comes to writing small chunks of data [5] and has less computational load on the processor of the computer using it, also is much faster at reading data than when accessing blocks of data of any size.

A cellular automaton is a relatively recent introduced simulation technique in the materials science. It was successfully used in the recrystallization phenomena of several types of steel [6] and memristor behavior [7]. Yu and Wright [8] were able to simulate nucleation and growth and predict microstructure evolution in phase change materials using cellular automata.

In this article it is used a simulation model based on the cellular automata technique to investigate the influence of defects in phase change materials on the switching speed.

2. The simulation model

The main difference between molecular dynamics and cellular automata is that instead of equations of motion and force fields in cellular automata the movement of the ingredients is governed by local rules. In this case larger systems can be simulated using low computational resources and it is obtained a general view of the investigated system dynamics.

The cellular automata simulation model consists of a two dimensional square lattice (grid) formed by $m \times m$ cells. Every cell interacts only with its first order von Neumann neighboring cells.

The simulation model was developed based on the concept of commuton which is the smallest unit that maintains the property of switching and was introduced by Popescu et al. [9]. Every cell contains a commuton and is characterized by the cell state, which can be 0 if the commuton is in the OFF state and 1 if the commuton is in the ON state, the cell coordinates on the grid, (x, y), where x is the row number and y is the column number, the cell energy, which stores the free energy of the commuton, and the cell threshold energy, at this energy the commutons switch from the OFF to the ON state.

The commutons exchange energy in a probabilistic manner, thus meaning that a commuton can absorb energy

from a higher energy comuton in his neighborhood or can transfer energy to a lower energy commuton from his neighborhood. The simulation starts with a grid filled with commutons in the OFF state (zero free energy), then an energy (which can be optical, electrical or thermal energy) pulse is applied on the grid by randomly selecting a commuton and increasing his energy by the pulse energy. After the energy pulse is applied, the energy is dissipated in his neighborhood with respect to the probabilistic rules and is checked if there are commutons that collected the required energy to switch in the ON state. Finally, the formation of the percolation path is checked, and then another pulse of energy is applied on the grid and so on. This cycle continues until the entire material switched, meaning that a cluster of ON commutons is connecting the top and bottom electrodes.

A detailed description of the model is presented in [10]. The validity of this model was demonstrated by applying it to $Ge_2Sb_2Te_5$ and successfully reproducing the abrupt drop in material resistance with the increase of the temperature at around 150 °C.

The switching process in the ferroelectric memory, at nanoscale, was visualized using a high-resolution transmission electron microscope [11]. When it was applied the electrical field to switch the state of the memory device, it was observed that the nucleation starts in several random places inside the material. Those nucleation points increase, suddenly merging and switching the entire material.

In a previous study [12] it was shown that the cellular automata model developed by us generates a behavior similar to the switching process in the ferroelectric memory. The crystallization process begins with the formation of the nuclei of ON commutons, these nuclei merge and form stable clusters. The evolution of crystallization takes place through the connection of the clusters and formation of the percolation path.

3. Results and discussion

In order to investigate the influence of defects on the percolation cluster size, there were used grids of various sizes (25×25, 50×50, 75×75, 100×100 and 125×125) and different percents of defects in the material, in the range of 0 – 40% defects. If we consider that the size of a commuton is comparable to the rock salt crystalline lattice of $Ge_2Sb_2Te_5$ of 6 Å, then the simulated area size is ranging from 1.5×1.5 nm^2 to 75×75 nm^2.

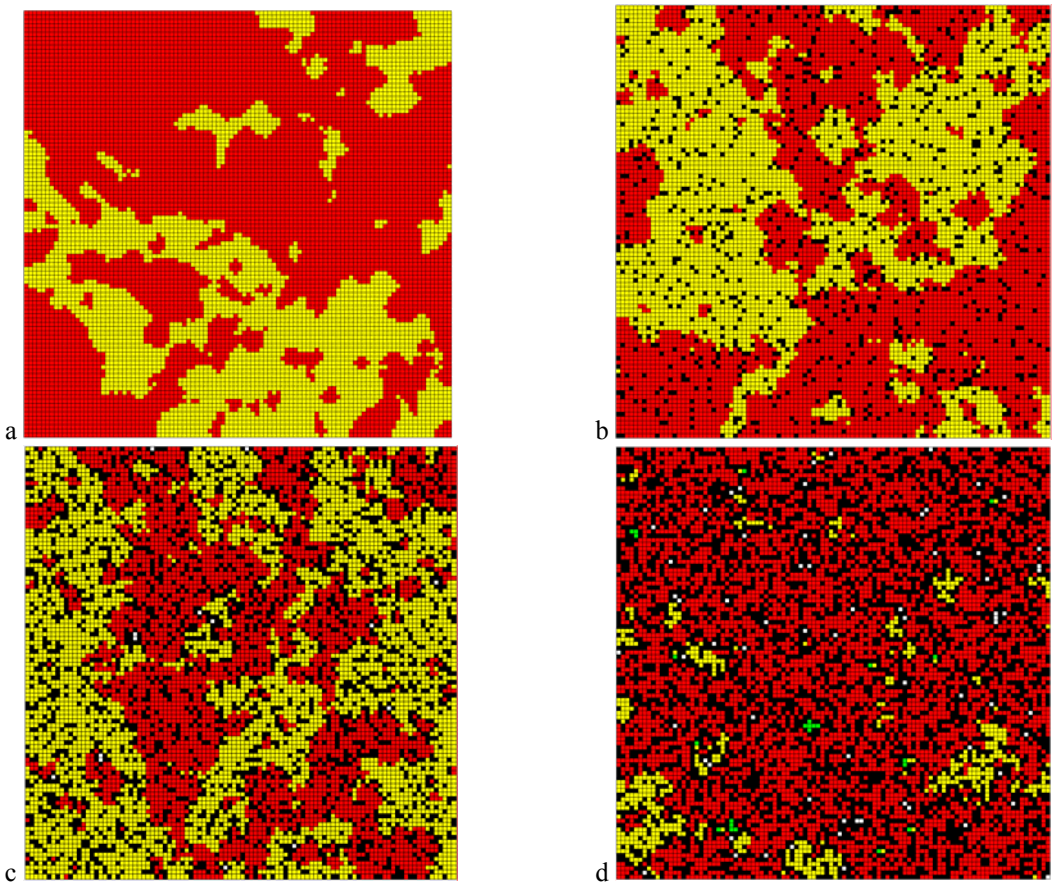

Fig. 1. Formation of the percolation path for a system of 100×100, with various percents of defects a) 0% b) 10% c) 25% d) 40%. Black squares are defects, white squares are commutons with zero free energy, green squares are commutons with the free energy between zero and half of the threshold energy, yellow squares are commutons with the free energy between half of the threshold energy and the threshold energy and red squares (ON commutons) are the commutons with the energy higher than the threshold energy. At 40% defects even if almost all the commutons are in the on state (except the ones surrounded by defects) the percolation path is not formed.

A defect is a vacancy that prevents the commutons from exchanging energy because it cannot absorb or transfer energy. The defects are randomly distributed on the grid at the beginning of the simulation.

The pulse energy for all the simulations was equal to the threshold energy of a single commuton. There were performed 20 simulations for every grid size and every percent of defects and the results were averaged. The standard deviation was less than 10% for all cases.

In Fig. 1 it can be seen the final state of a system, with a grid size of 100×100 and different percents of defects, where the percolation path is formed.

It can be observed that the percolation cluster size has a minimum around 25% defects (Figure 2). Increasing the number of defects from 0 to 25%, reduces the number of configurations accessible to the system and so, the energy given to the system is more efficiently used. Around 25% is reached the optimum tradeoff between the number of defects and speed of switching. By increasing further the number of defects, the state space further decreases such that it takes longer and longer to reach a state in which the percolation path is formed. This state becomes unreachable at 40% defects, because the randomly distributed defects form a barrier that prevents the percolation cluster from connecting the electrodes. This property is found for all sizes of the studied systems.

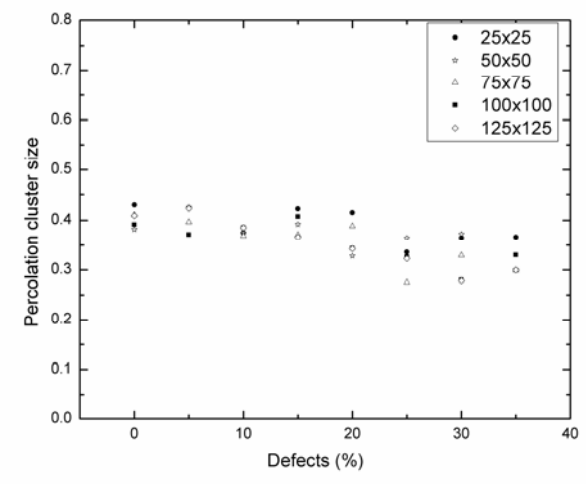

Fig. 2. Variation of the percolation cluster size as a function of the percent of defects

4. Conclusions

The switching phenomena from phase change materials can be simulated using simple, local rules that evidence the properties of the commutons which cannot be revealed by molecular dynamics.

By investigating the effect of defects on the switching speed it can be concluded that the defects introduced in the material have an enhancing effect over the rapidity of switching. This effect is largest at around 25% defects. However, one should be careful with the percent of defects introduced in the material because at 40% defects the switching of the material is totally blocked. These results are similar to those obtained by Wuttig et. al [13]. They have computed the formation energy of defects in the case of Ge—Sb—Te alloy using ab-initio calculations.

These findings offer the possibility to design new phase change materials and devices with better switching properties through the deliberate introduction of an optimal percent of defects into the material.

Acknowledgement

This work was financial supported by the Ministry of the Education, Research, Youth and Sports through the Project CNMP no. 12089/2008.

References

[1] McKinsey Global Institute report, www.mckinsey.com, (2011).
[2] G. I. Meijer, Science **319** (5870), 1625 (2008).
[3] S.R. Ovshinsky, Phys. Rev. Lett. **21** (20), 1450, (1968).
[4] M. Wuttig, N. Yamada, Nature Materials. **6**, 824 (2007).
[5] A. Akel, A. M. Caulfield, T. I. Mollov, R. K. Gupta, S. Swanson, Proceedings of the 3rd USENIX conference on Hot topics in storage and file systems, pp. 1-5, (2011).
[6] M. Qian, Z. X Guo, Materials Science and Engineering: A, **365**(1-2), 180 (2004).
[7] A. Adamatzky, L. Chua, arXiv:1111.2940v1 (2011).
[8] W. Yu, C.D. Wright, J. Univ. Sci. Tech. Beijing **15** (4), 444 (2008).
[9] M. Popescu, A. Velea, A. Lőrinczi, F. Sava, J. Ovonic Res. **5**(2), 27 (2009).
[10] A. Velea, Journal of Non-Crystalline Solids, **357**(14), 2626 (2011).
[11] C. T. Nelson, P. Gao, J. R. Jokisaari, C. Heikes, C. Adamo, A. Melville, S.-H. Baek, C. M. Folkman, B. Winchester, Y. Gu, Y. Liu, K. Zhang, E. Wang, J. Li, L.-Q. Chen, C.-B. Eom, D. G. Schlom, X. Pan, Science, **334(**6058), 968 (2011).
[12] A. Velea, Digest Journal of Nanomaterials and Biostructures, **5**(4), 1023 (2010).
[13] M. Wuttig, D. L. Sebrink, D. Wamwangi, W. Wełnic, M. Gilleßen, R. Dronskowski, Nat. Mater. **6**, 122 (2007).

*Corresponding author: velea@infim.ro