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SIMULATION OF PHASE CHANGE MATERIALS USING CELLULAR AUTOMATA

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The most promising media for rewritable applications are the phase change materials [1]. For the modelling of the phase transition processes in phase change materials was used the minimum switching unit called "commuton" [2]. A commuton is a minimum cluster of atoms that supports a reversible change from OFF to ON state under the influence of an external applied energy pulse. It was developed a bidimensional model based on the cellular automata approach [3] to predict switching behavior in a $Ge_2Sb_2Te_5$ phase change chalcogenide film. The formation of the percolation paths as a function of phase change induced in commutons can explain the switching phenomenon. The percolation thresholds of the switching were calculated for different sizes of the simulated system and the percolation kinetics was investigated.

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1. Introduction

Phase change materials present a reversible change from an amorphous (OFF) to a crystalline (ON) state by applying an appropriate external excitation. Even if these materials were studied more than 40 years the exact processes at atomic scale are still incompletely understood.

Popescu et al. suggested in [4] that the switch from the amorphous to crystalline state is not necessary and proposed a transition from an amorphous, disordered, state to a more ordered state, not necessary crystalline.

Molecular dynamics modeling leads to improved accuracy in the simulations, but suffer from important technical limitations in the simulation time and simulated system size. A novel modelling approach of phase-transition processes in phase change materials is related to the probabilistic cellular automata (CA) models [5, 6]. The CA models, could be very drastic in their approximations, but are able to offer a general view on global issues such as thermodynamics and dynamics of the simulated systems. They offer a complementary approach to the direct simulation of atomic scale models. These models use limited computational resources leading to an efficient simulation tool that can be related to optical, thermal, and electrical processes that appear in phase change materials.

2. The Cellular Automata Model

Popescu et al. defined in [2] the smallest unit that preserves the property of switching in memory materials called commuton (Fig. 1). In this article it is used the concept of commuton to build a cellular automata model for simulating the percolation process that appears in phase change materials.

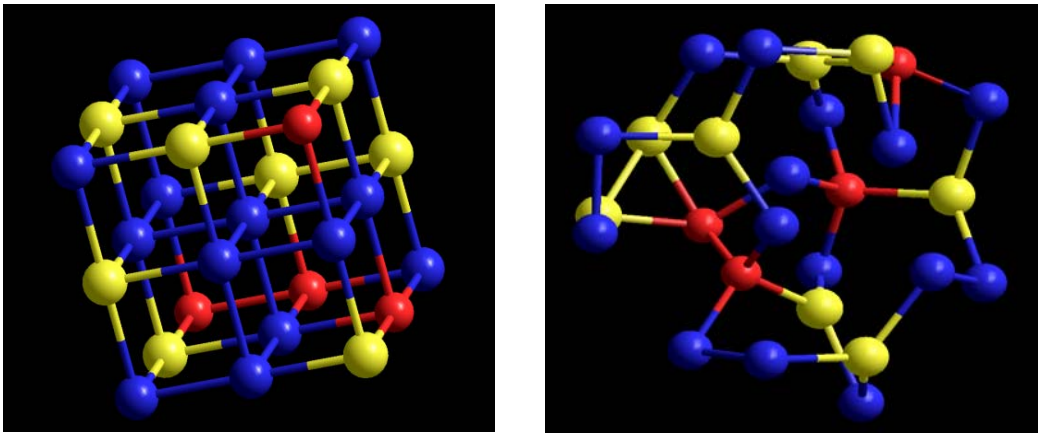

Fig. 1. The commuton a) Crystalline state (ON state) b) Amorphous state (OFF state)

The rules that govern the behavior of the cells are local, involving only a cell and those cells in its neighborhood. The cellular automata simulation model consists of a two dimensional square lattice (grid) formed by $m \times m$ cells. The interaction with the walls was neglected.

The first order neighbors of a cell, *i*, is composed of four adjacent cells, *j*, called the von Neumann neighborhood (Fig. 2). Every cell contains a commuton and is characterized by the following set of parameters:

- the cell state, *s*, is an integer 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, *e*, is also an integer which stores the free energy of the commutons;
- the cell threshold energy, e_{th}, at this energy the commutons switch from the OFF to the ON state.

The steps of the main program are the following:

1. Application of the energy pulse;
2. Dissipation of the input energy on the grid in a probabilistic manner;
3. Checking the switching of commutons;
4. Checking the formation of percolation;
5. Recording the attributes of the simulated system;

		j		
	j	**i**	**j**	
		j		

Fig. 2. von Neumann neighborhood of cell i

A detailed description of the model is presented in [7].

3. Results and discussion

In order to investigate the influence of the simulation area on the switching parameters we used in simulation grids of various sizes and various energy of the pulses.

In Fig. 3 one can see the percolation path for the following grid sizes: a) 50 × 50 cells, b) 75 × 75 cells, c) 100 × 100 cells, d) 150 × 150 cells e) 200 × 200 cells. The energy of the pulse is 10 e_{th} for every simulation.

If we consider that the size of a switching unit (commuton) is equal to the rock-salt lattice crystalline $Ge_2Sb_2Te_5$ of 6.00 Å, then the simulated grid corresponds to a real area of 30 × 30 nm^2, 45 × 45 nm^2, 60 × 60 nm^2, 90 × 90 nm^2 and 120 × 120 nm^2 of $Ge_2Sb_2Te_5$ thin film.

The crystallization process begins with the formation of nuclei of ON commutons, these nuclei interact one to another and forms stable clusters. The evolution of crystallization takes place through the connection of the clusters. The percolation occurs when is formed a path of connected clusters of ON commutons which cross the entire grid. The percolation it is analyzed only between upper and bottom electrodes.

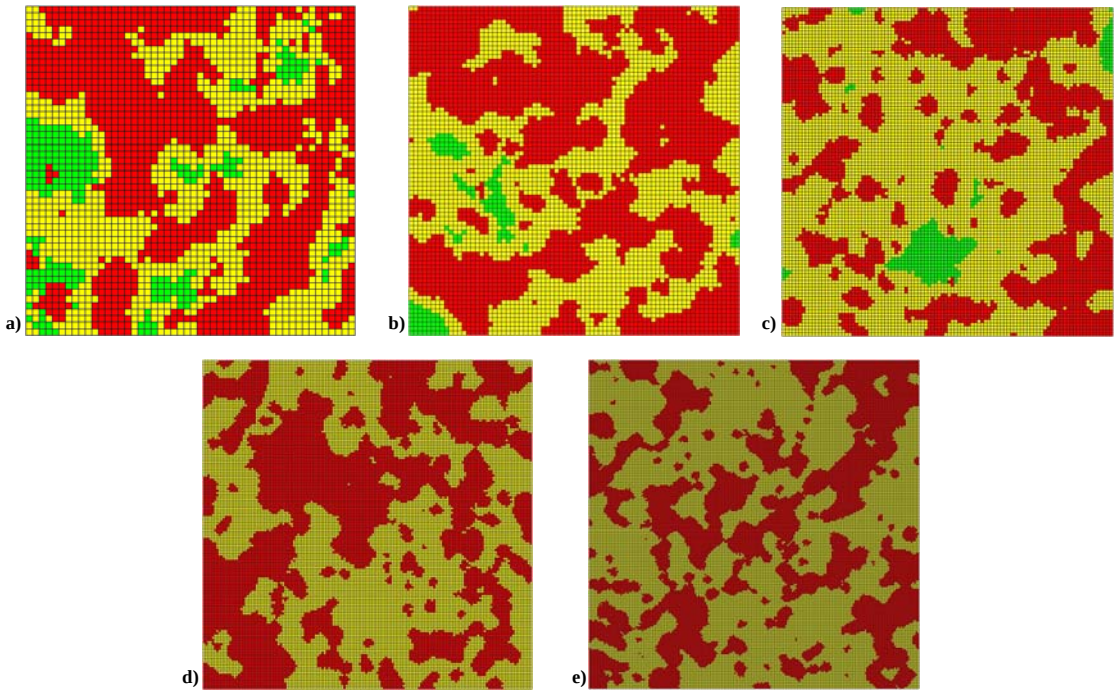

Fig. 3. The percolation threshold for various grid sizes using a pulse of energy of 10 e_{th} (10 times greater than the threshold energy of every commuton) (green=commutons with free energy between 0 and $e_{th}/2$, yellow=commutons with free energy between $e_{th}/2$ and e_{th}, red=commutons with free energy higher or equal to e_{th}) a) 50 × 50 cells; b) 75 × 75 cells; c)100 × 100 cells; d) 150 × 150 cells e) 200 × 200 cells.

The percolation thresholds are presented in Table 1. For every grid size and every energy of the pulse the simulation process has been run 10 times. The percolation threshold has been estimated by averaging the values got in the simulations and the errors were calculated. The percolation threshold is almost constant within the range of 0.4 ÷ 0.5 when the area of the simulated system changes and seems to decreases slowly with the increase of the energy of the pulse.

Table 1: Percolation thresholds for various sizes of the grid and various energies of the pulses

Grid size	Pulse energy				
	1 e_{th}	2 e_{th}	3 e_{th}	5 e_{th}	10 e_{th}
50×50	0.49±0.11	0.38±0.13	0.41±0.12	0.40±0.15	0.38±0.09
75×75	0.44±0.09	0.45±0.13	0.40±0.09	0.38±0.13	0.38±0.12
100×100	0.48±0.13	0.41±0.07	0.42±0.11	0.34±0.09	0.37±0.16
150×150	0.51±0.13	0.43±0.14	0.38±0.11	0.40±0.14	0.33±0.09
200×200	0.39±0.10	0.44±0.18	0.39±0.10	0.39±0.12	0.36±0.14

Fig. 4 shows the variation of the number of clusters of ON commutons, for various system sizes. One observes that the number of clusters increases rapidly until reaches a maximum. This stage corresponds to the formation of small, short lived clusters. In the second stage, the number of clusters drops abruptly, which means that a critical cluster size has been reached. These clusters are more stable, long lived and they have a greater probability of growing and merging. The third stage corresponds to the tail of the curve, where, there are still few smaller clusters left that will finally merge with the cluster that forms the percolation path covering the whole system.

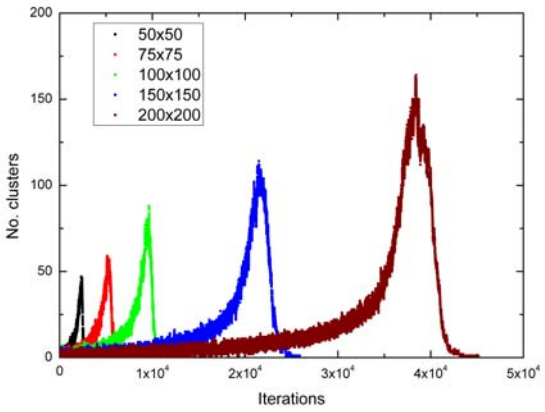

Fig. 4. Variation of the number of clusters of ON commuton as a function of time for various grid sizes

Fig. 5 shows the increase of the crystalline fraction as a function of time, for various energies of the pulses. The crystalline fraction is defined as the number of ON commutons divided by the total number of commutons in the simulated system. After an initial slow period of crystallization, the fraction of the ON commutons has an abrupt increase until reaches saturation when the whole system is switched. This behavior is in close connection to the clusters dynamics shown in Fig. 4. The crystallization process of $Ge_2Sb_2Te_5$ is very sensitive to the changes of the energy of the pulse. By increasing the energy of the applied pulses to the system, the switching time increases significantly.

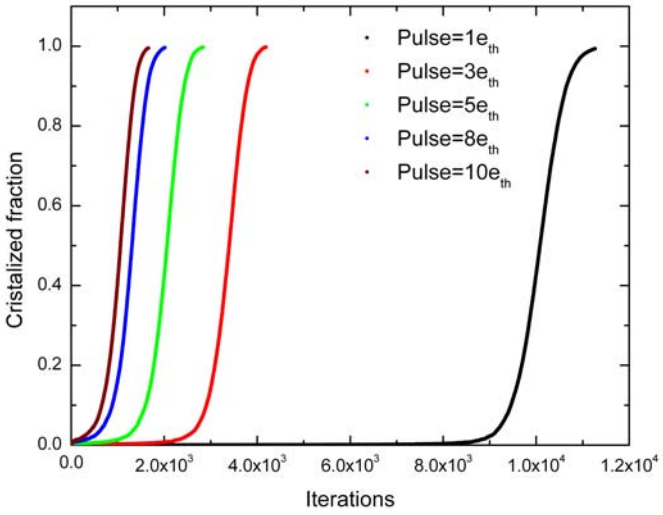

Fig. 5. Evolution of crystallized fraction of commutons for various energies of the pulse

4. Conclusions

It was demonstrated that the complex behavior of the phase change materials can be simulated using simple, local rules that evidence the properties of the phase change materials which cannot be revealed by molecular dynamics because of the limited size of the simulated systems.

The $Ge_2Sb_2Te_5$ system was modelled using a 2D cellular automata approach. The evolution of the switching process was investigated based on the dynamics of the commuton clusters for various sizes of the system and various energies of the applied pulses. The formation of percolation paths of ON commutons which crosses the whole system explains the switching phenomena.

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