

# Gillespie type cellular automata approach for phase-change device modelling

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## Abstract

A Gillespie type cellular automata (GCA) simulator [1] capable of spatio-temporal modelling of the amorphization and crystallization behaviour in phase change devices, such as random access memory cells (PCRAM) during the complex annealing cycles is presented. The model is based on the bulk, electrostatic and surfaces energies to produce rates of nucleation, growth and dissociation of crystallites made of "monomers". To deal with the events during the phase change transformation a stochastic Gillespie type algorithm is used. The phase change dynamics are coupled with the electrical and thermal fluxes to study the switching dynamics associated with the reset and set operations.

## 1. INTRODUCTION

Several methods have been used to model crystallization in phase-change alloys, such as the Johnson–Mehl–Avrami–Kolgomorov model (JMAK), nucleation and growth models, rate equation and ab-initio models. The GCA simulator approach is potentially capable to span from scales between atomistic methods, as DFT, to bulk scale methods, such as the JMAK formalism. The model has the thermodynamic features of rate equation and the elements of probabilistic cellular automata. It also uses a Gillespie algorithm for time stepping, allowing fast simulation of complex spatial and temporal annealing (cooling/heating) cycles in the operation of real devices.

## 2. DESCRIPTION OF THE MODEL

The operations in phase change devices involve an electro-thermal process. As a consequence to completely understand the physical processes in electrical data storage applications, it is necessary to have a complete coupled physical model consisting of three different sub-models, electric thermal and phase transformations involved in writing, erasing and reading data.

*Electric and thermal models.* The current density distribution through the material is modelled with the Laplace equation (1) and the temperature distribution throughout the material is obtained by the solution of the heat transfer equation(2)

$$\nabla \cdot (\sigma \cdot \nabla V) = 0 \quad (1)$$

$$\rho C_p \left[ \frac{\partial T}{\partial t} \right] - K \cdot \nabla^2 T = Q = E \cdot J \quad (2)$$

where  $\rho$  is the material density,  $C_p$  is the specific heat capacity per unit mass,  $K$  represents the thermal conductivity of the material,  $E$  and  $J$  the electrical field and the current density respectively and  $Q$  is the heat source per unit volume generated inside the material.

The behaviour of electrical conductivity in the amorphous state is modelled including temperature and field dependence. The electrical conductivity of crystalline chalcogenides behaves according to an Arrhenius relation [2]. The values of the thermal and electrical conductivity are assumed to switch from the amorphous to crystalline value, when the crystal fraction of the material reaches the percolation threshold, typically 15% [3].

*Phase-change model.* A homogeneous and isotropic material on a rectangular lattice is considered. The state of the material is defined on the discrete regular lattice of points. Each grid point  $(i, j) \in G$ , is described by the quantities:

- a)  $r_{ij}$  is defined as the phase, that can be amorphous (0) or crystalline (1).
- b)  $\Phi_{ij}$  is an orientation variable in a range  $0$  to  $\pi$ .

The temporal evolution is based on a stochastic model, which provides an estimate of rates of the possible local changes to the state of the system and employs a Gillespie algorithm that generates time steps corresponding to the highest rate which requires an update.

In the GCA approach [1], the following events in each site  $(i, j)$  are possible :

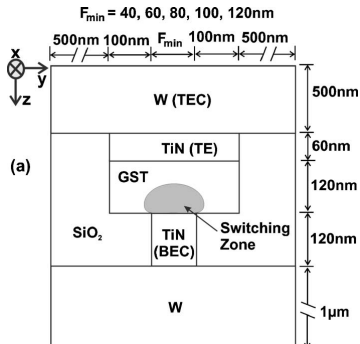
*Nucleation:* A site  $(i, j)$  and an adjacent site  $(k, l)$ , changes from amorphous to crystalline to form a single crystal at a rate  $C_{ij}^{nu}$ .

*Growth:* A site in amorphous state becomes attached to an adjacent crystal of orientation  $\Psi$  with rate  $C_{ij}^{gr}$

*Dissociation:* A site which is originally crystalline, dissociates from the crystal of which it was part and becomes amorphous at the rate  $C_{ij}^{dis}$  assuming a new random orientation.

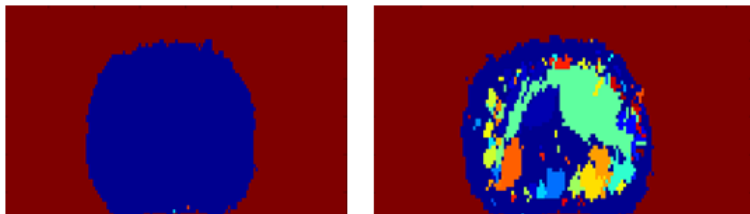
### 3. RESULTS FOR PCRAM

The transitions in PCRAM are accomplished by heating of the material via electrical pulses. For amorphization processes of the crystalline phase (RESET operation) the material is heated above its melting point and rapidly quenched. For the re-crystallization of the amorphous material from the reset operation, the material is heated to a temperature between the glass transition and the melting temperature via a moderate electrical pulse of low amplitude and longer duration.



Cross sectional view of the vertical PCRAM cell used in the set and reset operations taken from [4].The cell consists of a W top electrode contact (TEC), TiN top electrode (TE), a GST phase change layer, TiN bottom electrode contact(BEC), and W plug. The current flows vertically from TEC through GST to BEC and the reversible phase transitions occurs at the GST-BEC interface. The switching current is mainly determined by the BEC contact size.

The reset operation (crystalline to amorphous) is simulated with the GST initially in fully crystalline state. During the reset operation a pulse of 1.5 V, and duration 40 ns is used. The set operation (amorphous to crystalline) a portion of the GST material near the GST - BEC is initially in the amorphous state. For this operation a pulse of 0.8 V and duration 200 ns is applied to the PCRAM cell. The figure below shows the phase distribution for both operations.



(Left) Phase distribution throughout the material at  $t=40\text{ns}$ . The amorphous is in blue and in red is the portion of the material in crystalline state. (Right) Phase distribution throughout the material at  $t=200\text{ ns}$ . The different colors inside the amorphous dome represent different crystals.

### ACKNOWLEDGEMENTS

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