

A Cellular Automata Approach for the Simulation and Development of Advanced Phase Change Memory Devices

Submitted by

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Abstract

Phase change devices in both optical and electrical formats have been subject of intense research since their discovery by Ovshinsky in the early 1960's. They have revolutionized the technology of optical data storage and have very recently been adopted for non-volatile semiconductor memories. Their great success relies on their remarkable properties enabling high-speed, low power consumption and stable retention. Nevertheless, their full potential is still yet to be realized.

Operations in electrical phase change devices rely on the large resistivity contrast between the crystalline (low resistance) and amorphous (high resistance) structures. The underlying mechanisms of phase transformations and the relation between structural and electrical properties in phase change materials are quite complex and need to be understood more deeply. For this purpose, we compare different approaches to mathematical modelling that have been suggested to realistically simulate the crystallization and amorphization of phase change materials. In this thesis the recently introduced Gillespie Cellular Automata (GCA) approach is used to obtain direct simulation of the structural phases and the electrical states of phase change materials and devices. The GCA approach is a powerful technique to understand the nanostructure evolution during the crystallization (SET) and amorphization (RESET) processes in phase change devices over very wide length scales. Using this approach, a detailed study of the electrical properties and nanostructure dynamics during SET and RESET processes in a PCRAM cell is presented.

Besides the possibility of binary storage in phase change memory devices, there is a wider and far-reaching potential for using them as the basis for new forms of arithmetic and cognitive computing. The origin of such potential lies in a previously under-explored

property, namely accumulation which has the potential to implement basic arithmetic computations. We exploit and explore this accumulative property in films and devices. Furthermore, we also show that the same accumulation property can be used to mimic a simple integrate and fire neuron. Thus by combining both a phase change cell operating in the accumulative regime for the neural body and a phase change cell in the multilevel regime for the synaptic weighting an artificial neuromorphic system can be obtained. This may open a new route for the realization of phase change based cognitive computers.

This thesis also examines the relaxation oscillations observed under suitable bias conditions in phase change devices. The results presented are performed through a circuit analysis in addition with a generation and recombination mechanism driven by the electric field and carrier densities. To correctly model the oscillations we show that it is necessary to include a parasitic inductance.

Related to the electrical states of phase change materials and devices is the threshold switching of the amorphous phase at high electric fields and recent work has suggested that such threshold switching is the result of field-induced nucleation. An electric field induced nucleation mechanism is incorporated into the GCA approach by adding electric field dependence to the free energy of the system. Using results for a continuous phase change thin films and PCRAM devices we show that a purely electronic explanation of threshold switching, rather than field-induced nucleation, provides threshold fields closer to experimentally measured values.

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