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Modeling of data retention statistics of phase-change memory with confined- and mushroom-type cells

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ABSTRACT

Data retention statistics of phase-change memory with two representative cell schemes, confined and mushroom cells, were investigated using phase-field method that can correctly model successive nucleation events and their growth, simultaneously. Several directions of cell structure engineering are suggested. An interesting point is that reducing only one lateral dimension below a characteristic length can improve the data retention. Most importantly, it was found that the cumulative distribution of the retention time is Weibull for the mushroom cells while that is lognormal for the confined cells.

1. Introduction

Data retention is a key reliability issue for all nonvolatile memories (NVMs) because they are not perfectly nonvolatile. Industrial specification is usually ten years at around 80 °C, meaning that once data are recorded they should last at least for ten years at such operating temperature. Manufacturers always need to predict the retention time, t_{RET}, along with other device characteristics for the next-generation technology development. Moreover, in case of the data retention, the experimental test cannot be performed for ten years in the product development. Usually the t_{RET} value at 80 °C is extrapolated from the tests at higher temperatures using the Arrhenius equation. A baseline is that the data loss mechanism is a kind of thermally activated processes, which turned out to be true in most cases. Nonetheless, correct models that can properly capture essential physics for different NVMs are of great necessity.

Phase-change memory (PCM) is a matured technology compared to other new memories such as resistive random access memory (ReRAM) and spin-torque transfer magnetic random access memory (STT-MRAM), both of which are still under research stage. The volume production of the PCM is expected very soon. At present, two applications are under consideration. One is the storage class memory (SCM) to make up the latency between DRAM and storage (solid-state drive or hard-disk drive) [1]. The other is the neuromorphic computing where the PCM cells are used as synapses [2,3]. Needless to say, the data retention must be guaranteed to some degree in both applications.

The PCM adopts a chalcogenide material, typically, $Ge_2Sb_2Te_5$ (GST225) with some additives, as its recording material. In the field of electronic devices, the term, GST, is frequently used as a generic name for chalcogenide materials that reversibly transform between conductive crystalline and resistive amorphous phases, i.e. low and high resistance states, corresponding to zero and one. Switching from one to the other is done by Joule heating of the active material (self-heating) or a heating element, usually called a bottom electrode contact (BEC), which depends upon the cell geometry and materials. Crystal-to-amorphous transition (reset) occurs by a short high-power pulse (20–50 ns) while amorphous-to-crystal transition (set) occurs by a long moderate-power pulse (>100 ns). The former and the latter resemble quenching and annealing in materials processing, respectively.

In general, the retention failure of NVMs is essentially related to thermodynamically spontaneous phenomena. For example, a NAND flash cell with a high threshold voltage (V_{th}) contains many electrons in its floating gate or its charge trapping layer. The electrons gradually leak from the cell by absorbing ambient thermal energy. As a result, the V_{th} gradually decreases, leading to the retention failure. In case of the PCM, the crystallization that is also a spontaneous process is the root-cause. The Gibbs free energy of the crystalline state is lower than

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that of the amorphous phase. Crystalline nuclei successively appear and grow, that is called nucleation and growth (NG). At a moment, the crystalline domains are connected between top and bottom electrodes. Correspondingly, the cell resistance decreases from the reset resistance (R_{reset}) and finally reaches the set resistance (R_{set}), that is, the retention failure. The crystallization kinetics must be slow enough in order to meet the t_{RET} specification. In this reason, many efforts have been made to increase the stability of the amorphous state by material engineering [4–6]. The data retention time is also affected by the cell geometry such as shape and size.

This paper presents a thorough investigation on t_{RET}-distributions for two representative cell schemes that are confined and mushroom cells. We presented 3D phase-field method (PFM), a mesoscale simulation, combined with stochastic nucleation seeding in our prior reports where only confined cells with cubical GST region and their isotropic scaling were investigated [7–9]. However, the cubical GST geometry might not be practically used in the fabrication process [10]. Therefore, we should turn our focus to the noncubical GST cell that is more realistic. The dependence of the t_{RET}-distribution on the cell scheme and the cell dimensions will be discussed. We will show two central results: one is that the contact area between GST and electrode and the distance between top and bottom electrodes are the key factors for both cells, and the other is that the t_{RET}-distribution of the mushroom cell is Weibull while that of the confined cell is lognormal.

2. Theory and simulation method

2.1. Crystallization in nanoscale systems

The crystallization occurs via NG as mentioned. Atoms in an amorphous phase move around constantly like “liquid” (but very slowly). At an instant, several atoms form a small crystalline cluster, that is, a crystallite with a volume, V, and a surface area, A. The volume free energy decreases by $-\mathrm{V}\Delta G$ and the interface free energy increases by $+\mathrm{A}\gamma$ where ΔG and γ are the bulk free energy difference [J/cm^3] and the interface energy [J/cm^2] between amorphous and crystalline phases, respectively. The corresponding change of the total free energy is the summation of two contributions.

$$\Delta G_{total} = -\mathrm{V}\cdot\Delta G + \mathrm{A}\cdot\gamma \tag{1}$$

In case of a small crystallite, the interface energy increase dominates the bulk free energy decrease. Thus, it disappears immediately after the formation of the crystallite because the total free energy of the system increases ($\Delta G_{total}>0$). Conversely, a large crystallite is stable because the bulk free energy is dominant ($\Delta G_{total}<0$). The stable crystallite starts to grow, resulting in a further decrease of the total free energy. The occurrence of the stable crystallite is called the nucleation. There exists a critical size, a^*, for nucleation determined by the condition, $(\mathrm{d}\Delta G_{total}/da)_{a=a^*}=0$, where a is the size of the crystallite. The nucleation rate is a rate per volume, I_N [cm$^{-3}\cdot$s^{-1}]. Each nucleus is assumed to grow at a constant speed, V_G [cm$\cdot$s^{-1}], that is called, the growth velocity. The macroscopic crystallization kinetics including all these effects is summarized by the Johnson–Mehl–Avrami–Kolmogorov (JMAK) equation that yields the “S-curve” for transformed fraction as a function of time, X(t) [11].

$$\mathrm{X(t)} = 1 - \exp(-\mathrm{b}t^n) \tag{2}$$

where $\mathrm{b}=(1/3)\pi V_G^3 I_N$ and $\mathrm{n}=4$. Steady-state nucleation ($I_N=$const.) is assumed for an infinitely large 3D sample. Note that Eq. (2) is deterministic with no statistical deviation. Both of I_N and V_G have strong temperature dependence because the macroscopic NG occurs by thermally activated atomic displacements.

However, the assumption of the infinitely large sample is problematic for our nanoscale PCM cells. When it comes to smaller samples than a certain limit, Eq. (2) need be modified to include the cell size dependence, which was done before [9,12]. More importantly, the statistical deviation in the kinetics becomes larger for smaller samples due to the increased stochastic nature of the nucleation. Such size effects are clearly observed in the modern PCM cells where the t_{RET}-distribution becomes wider upon scaling-down [7,13].

The t_{RET}-distribution of a cell array includes both extrinsic and intrinsic variations [14]. The extrinsic variation is related to the difference of dimensions, compositions, and interface quality between the cells. The intrinsic variation comes from the random nature of the nucleation and thus occurs even for identical cells. The extrinsic portion can be reduced by improving the process while the intrinsic portion cannot be improved. Separating two contributions from a measured distribution can provide the limit for reducing variations. Knowing the limit is important for efficient development in industry but it is practically impossible solely by experiments. So the physical modeling must be accompanied.

2.2. Simulation of nucleation and growth using phase-field method

The NG produces intricate nanoscale phases in three-dimensions and the time-scale varies from nanoseconds to years depending upon temperature. This relatively large size and long time-scale are intractable with ab initio or classical molecular dynamic calculations. Conversely, current commercial softwares such as device simulators and multiphysics tools cannot deal with such dynamically changing complex geometry. In general, the finite element method is inefficient in this case because remeshing on changing geometry is necessary at every time step. Therefore, a different simulation method is necessary. The phase-field method (PFM) is the right one.

The PFM calculates the geometrical evolution of the mixed phases (the amorphous and crystalline phases in case of our PCM) toward reducing the total free energy as shown in Fig. 1. Similarly to the classical nucleation and growth theory discussed in Section 2.1, the PFM also describes the total free energy as a sum of the bulk free energy and the interfacial free energy. A different thing is that all the energies are expressed as a function of a position-dependent continuum field that is related to the local phase. The field is usually called an order parameter in the PFM. For a GST cell, an order parameter, $\eta(\vec{r})$, has a value of zero and one inside and outside crystalline regions, respectively, as shown in Fig. 1. Please note that the order parameter is dimensionless and gradually changes across interfaces, which is called diffuse interface description [15].

The bulk free energy density, $f(\eta)$, should be a double well potential that has minima at $\eta=0$, 1 and a barrier between the minima. The free energy of the amorphous phase should be higher than that of the crystalline phase such that $f(1)>f(0)$. We constructed a formula that reflects all above points and whose shape is shown at the upper right corner of Fig. 1.

$$f(\eta) = \frac{W}{4}\eta^2(1-\eta)^2 + \eta^3(10-15\eta+6\eta^2)\cdot\Delta G \tag{2}$$

where W determines the potential well height between two phases and ΔG determines the free energy difference between crystalline and amorphous phases. Please note that another form of $f(\eta)$ may be taken as long as it satisfies the given physical requirements. The W is a calibration parameter while the ΔG is a physical parameter expressed as $\Delta G=\Delta H_f(1-T/T_m)$ where ΔH_f denotes the enthalpy of fusion and T_m is the melting point of the GST [16]. When temperature reaches T_m, both minima has the same function value of zero, meaning that crystalline and liquid phases can coexist. Amorphous is essentially (supercooled) liquid.

The gradient of the order parameter is nonzero only at diffuse interface regions. The nonzero gradient is utilized as the interface energy.