Driving forces of mass transport in phase change materials and their effect on device failures

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Various thermodynamic driving forces including electric-field, temperature gradient, mechanical stress, and concentrational gradient are considered to investigate the mass transport of $Ge_2Sb_2Te_5$ in phase change memory. The driving forces are systemically understood and quantified by the model study using a large symmetric and asymmetric bridge device and 1-dimentional simulation using finite difference method (FDM). The results showed that mechanical stress and concentration gradient induced atomic migration play as back driving forces to reduce the mass transport by electric field.

Key words: phase change memory, $Ge_2Sb_2Te_5$, mass transport, back force, immortal condition, etc.

1. INTRODUCTION

Phase change memory (PCM) has limits to use as a universal memory device because of its low cycling endurance. The endurance failures in PCM are caused by the composition change and void formation in phase change materials [1]. The compositional variation and the void formation are the results of the mass transport in phase change materials. In order to prevent these failures and improve the reliability of PCM, the origins of the degradation behaviors should be clearly identified. The failures can be predicted in specific operating conditions and various phase change materials from the failure mechanisms. However, the failure analysis is restricted in real PCM device due to the small size and the existence of various driving forces. We have used a simple symmetric bridge cell with large dimension, and investigated the mass transport in $Ge_2Sb_2Te_5$ (GST) by electromigration [2-3]. As for the thermodynamic driving forces for mass transport, various forces, such as electric-field, mechanical stress, temperature-, and concentration-gradient, are suggested. Electromigration in GST is well investigated and known as the driving force for atomic migration of constituent element. However, the effects of mechanical stress, temperature, and concentration change on atomic migration in GST have not been studied. Because these thermodynamic driving forces are generated during the device operation, the forces should be systemically studied to understand the mass transport in PCM. The stress and concentration gradient are caused by the electromigration, and the forces from them are opposite to the electromigration; these are back-driving forces. Because these back-driving forces depend on the dimension of diffusion path, the effect of back-driving force is critical on the mass transport in the real device. In the present work, we investigate the effects of the back-driving force on the mass transport in PCM using the finite-difference method (FDM).

2. EXPERIMENTS

The electromigration behavior of GST was investigated using an electrical-pulse-stressing to a 20μm-length-symmetric-bridge-type cell. The changes in concentration of elements were observed using wavelength-dispersive X-ray spectroscopy [2-3]. The results of electromigration were compared with the calculation by FDM, and back-driving forces were calculated. The system for the FDM was assumed to be one-dimensional. We calculated the changes in the number of constituent atoms in the i^{th} element from the incoming flux to the i^{th} elements and outgoing flux from the i^{th} elements. The changed values in number of atoms and stress in each element are used in the next iteration for the loop process. The output parameters are the number of constituent atoms in each element from anode to cathode. The calculation was conducted in 20μm-length and 100nm-length cells to investigate the effect of scaling.

3. RESULTS & DISCUSSION

We demonstrated related the atomic transport to each driving force by adding a driving force one by one and compared it with the experimental results. In the calculation considering only electromigration, the concentration of each element change abruptly and the accumulation atoms occurred only at the cell in contact the electrode. Because this concentration profile leads to a very large concentration gradient-induced driving force, this profile is unrealistic with respect to the experimental results. When the concentration gradient-induced driving force was also considered with electromigration, the concentration profile became very similar to experimental results. However, the amount of accumulated atoms at the electrodes is still too high, which induces large compressive stress. Figure 1(a)-(c) shows the calculated compositional profile by FDM after the pulse current stressing of 7 MA/cm^2 in consideration of electromigration, concentration gradient, and stress. The compositional profile of Ge, Sb, and Te is very similar to the experimental results presented in Fig. 1(d)~(f), which are observed by single-pulse-electrical stressing into the symmetric-bridge-type device [3]. This result indicates that the back-driving force should be considered in the analysis of mass transport in PCM. Mass transport produces the concentration gradient and stress gradient in a material as shown in Fig. 2. The directions of the driving forces due to the compositional change and stress are opposite to the vectorial sum of electromigration and thermomigration. They act as a back driving force to inhibit further degradation by mass transport. To estimate the mass transport behavior including the back-flux force in very short height like a real PCM devices, we employ the same FDM model in 100 nm-length cell. Figure 3 shows the mass transport with increase of duration time in 100 nm length. The compositional demixing is also occurred in the $Ge_2Sb_2Te_5$ by the electromigration. Figure 3(d) shows the differences of atomic concentration between the top electrode and the bottom electrode ($\Delta C_{TCE\text{-}BCE}$) to the duration time of reset pulse. The $\Delta C_{TCE\text{-}BCE}$ of Ge, Sb, and Te increase with the duration time, and barely change after 500 ns. The saturation of $\Delta C_{TCE\text{-}BCE}$ indicates that mass transport by electromigration does not occur in the phase change volume. The back-flux driving force due to the stress and concentration changes build up in the phase change volume, and become equal to the sum of the electromigration and thermomigration forces after 500 ns. The back-flux force from the stress and concentration depend on the dimensions of the system. The back-driving forces increase with the decreasing height of the phase change volume. Therefore, if the length of the line is reduced, the concentrational change in equilibrium also decreases.

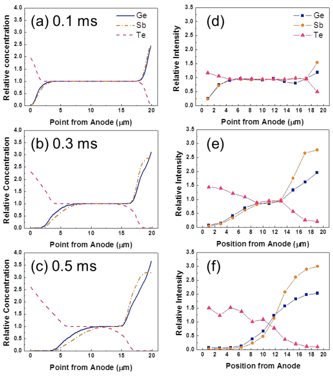

Figure 1. Comparison of composition profile after Electromigration between in FDM and in experiments.

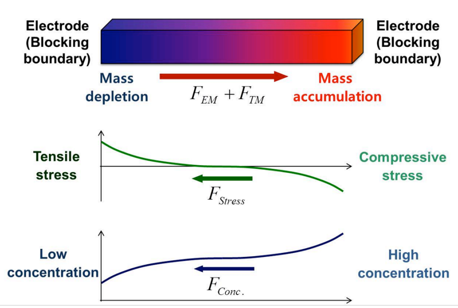

Figure 2. Back driving forces due to the generation of the stress and concentration gradient that results from electromigration and thermomigration.

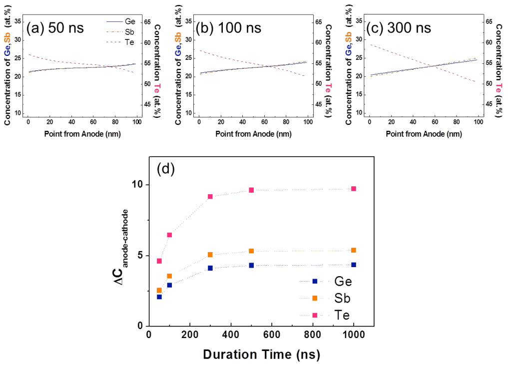

Figure 3. Composition change in 100nm-height PCM cell under current Stresssing with 10 MA/cm^2 to the duration time.

4. CONCLUSION

Based on this FDM calculation, we identified the suppression of mass transport in PCM due to the back-driving forces associated with the concentration- and stress-gradient. Mass-transport-induced endurance failure in PCM will be improved when the length or the thickness of the phase-change volume decreases.

REFERENCES

[1] K. Kim and S. J. Ahn, IEEE Reliability Physics Symposium Proceedings, **2005**, 157-162.
[2] T.-Y. Yang, J.-Y. Cho, and Y.-C. Joo, *Electrochem. Solid State Lett.* **13** (9), H321-H323 (2010).
[3] T.-Y. Yang, I.-M. Park, B.-J. Kim, and Y.-C. Joo, *Appl. Phys. Lett.* **95** (3), 032104 (2009).