

Structural relaxation related to resistance drift in amorphous GeTe thin films

F. Hippert^{a*}, J.-Y. Raty^{b,c}, F. d'Acapito^d, P. Montéléon^c, C. Sabbione^c,
N. Castellani^c, P. Kowalczyk^c, N. Bernier^c and P. Noé^c

- a. LNCMI (CNRS, Université Grenoble Alpes, UPS, INSA), Grenoble, France.
- b. Physics of Solids Interfaces and Nanostructures, Université de Liège, Belgium.
- c. Université Grenoble Alpes, CEA-LETI, Grenoble, France.
- d. CNR-IOM-OGG c/o ESRF, Grenoble, France.

*Francoise.Hippert@lncmi.cnrs.fr

Chalcogenide phase-change materials (PCM) such as $\text{Ge}_2\text{Sb}_2\text{Te}_5$ or GeTe alloys can be quickly and reversibly switched between an amorphous and a polycrystalline phase with very different optical and electrical properties [1]. This outstanding combination of properties led to their use first in optical and recently in resistive non-volatile memories. Resistive PCM memories are a promising candidate in order to replace the FLASH memories at technology nodes under 28 nm and to fill the gap between DRAM and NAND [2]. In a PCM memory, the amorphous or crystalline state of a small confined volume of the PCM is selected by application of a programming current pulse. One major issue in the development of PCM memories is to understand and reduce the resistance drift (resistance increase with time, i.e. with ageing) of the amorphous phase, especially for the development of multi-level cell storage technology. The origin of the resistance drift in chalcogenide phase-change glasses has been widely debated but no consensus emerged up to now on the nature of the structural relaxation occurring during ageing. *Ab initio* simulations of the amorphous GeTe phase [3] have suggested that the number of homopolar Ge-Ge bonds decreases with ageing. The Ge-Ge bonds are inherent to the presence of tetrahedrally bonded Ge atoms. The fully relaxed amorphous structure would be a Peierls-distorted structure consisting of 3-fold (distorted octahedral environment) Ge and Te atoms with only Ge-Te bonds. This ideal structure reminds that of the GeTe crystal structure but with much larger local Peierls distortions. In contrast with these predictions we observed from the analysis of Extended X-Ray Absorption Fine Structure (EXAFS) at the Ge K-edge [4] and Fourier-transform infrared (FTIR) spectroscopy that the number of Ge-Ge bonds increases upon ageing in amorphous GeTe thin films deposited by sputtering. One possible explanation of these results could be a clustering of the Ge atoms in amorphous GeTe upon ageing. Such a segregation is indeed found in Transmission Electron Microscope images of an aged film and confirmed by the excellent agreement found between the total structure factor measured by X-ray scattering and calculated by new *ab initio* simulations that include Ge segregation [5].

[1] S. Raoux and M. Wuttig, *Phase Change Materials: Science and Applications* (Springer Science & Business Media, New York, USA, 2009).

[2] A. Redaelli, *Phase Change Memory, Device Physics, Reliability and Applications* (Springer International Publishing AG, 2018).

[3] J.Y. Raty *et al*, Aging mechanisms in amorphous phase-change materials, *Nature. Com.* **6**, 7467 (2015); S. Gabardi, S. Caravati, G. C. Sosso, J. Behler and M. Bernasconi, Microscopic origin of resistance drift in the amorphous state of the phase-change compound GeTe, *Phys. Rev. B* **92**, 054201 (2015).

[4] P. Noé *et al*, Structural change with the resistance drift phenomenon in amorphous GeTe phase change materials thin films, *J. Phys. D: Appl. Phys.* **49**, 035305 (2016).

[5] P. Noé *et al*, to be published.