Structure, dynamical properties and topology of GST phase change materials.

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Ge-Sb-Te alloys (GST) have been successfully used as Phase Change Materials for data recording applications. They exhibit a unique collection of properties that make them adequate for high performance non-volatile RAM memories. Indeed, their crystalline phase(s) are extremely contrasted, both optically and electrically, against their easily generated amorphous phase(s).

Understanding the fast switching mechanisms and the amorphous phase properties remains however quite challenging. In particular, the stability of the amorphous phase against phase separation, recrystallization, and drift of the electronic properties with time and cycling remain problematic. In this work, we generate models of a series of amorphous GST alloys using DFT molecular dynamics and simulated annealing. The obtained structures are compared and generic patterns are described. A new algorithm to determine the topological constraints, based on the analysis of the fluctuations of interatomic bond lengths and bond angles, has been proposed and applied to seven alloy compositions in the GeSbTe phase diagram [1]. A constraint map could then be drawn for the whole ternary system. According to this, the most commonly used GST amorphous phases are shown to be in the stressed rigid region [1]. In order to estimate the effect of rigidity on the recrystallization temperature (Tc), we performed a similar study for Carbon and Nitrogen doped GeTe [2]. The increase of the number of constraints upon doping is shown to be correlated with an increase of the recrystallization temperature and a reduction of the low frequency, or floppy, vibrational modes [3]. The generality of this stabilization mechanism is finally tested on other systems.

[1] M. Micoulaut, J.Y. Raty, C. Otjacques, and C. Bichara, Physical Review B 81 (2010) 174206

[2] G. Ghezzi, J.Y. Raty, S. Maitrejean, A. Roule, E. Elkaim and F. Hippert, Applied Physics Letters, 99 (2011) 151906.

[3] J.Y. Raty, P. Noe, G.Ghezzi, S. Maitrejean, C. Bichara and F. Hippert. To be published.