H5. REWRITABLE DVD, RAM MEMORIES: BETWEEN THE ELECTRONIC STRUCTURE AND THE RECORDING ABILITY, NEUTRON SCATTERING SHED SOME LIGHT.

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Data storage and memory devices utilizing the optical and electrical properties of phase-change (PC) materials are important for multimedia applications[1]. The pseudo-binary chalcogenide compound $(GeTe)_2$-Sb_2Te_3 ($Ge_2Sb_2Te_5$) is one of the reference materials for commercial DVD-RAM (digital versatile disc-random access memory) because it presents good optical and electrical contrast.

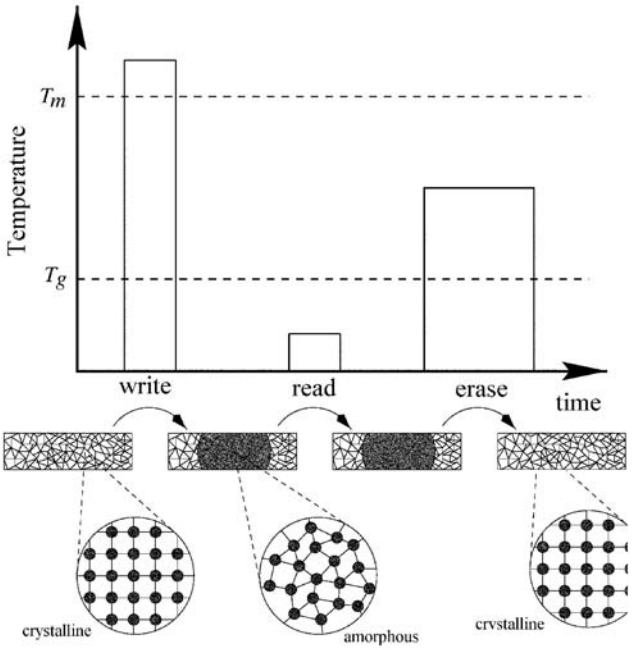

Figure 1: Write, read and erase sequence. T_g is the glass transition temperature and T_m is the melting temperature.

More precisely, the GeSbTe phases have the ability to easily crystallise and amorphise under the action of a laser pulse, basic process of commercial phase-change optical disks. During this reversible process, the crystal is locally melted to obtain an amorphous spot (crystal-liquid-amorphous transitions): this corresponds to the recording process. In a second time, this spot can be recrystallised (amorphous-crystal transition) by using a less intense laser beam, this is the erasing process (Fig. 1). The recrystallisation of the material is the slower process. In order to develop faster phase-change materials, it is necessary to understand the transformation mechanism and the structural origins of the phase change from amorphous to crystal.

A number of new materials for optical and electronic non-volatile pc-storage have been identified by trial and error [1]. Recently, microscopic models of the amorphous and crystalline states have been suggested to explain the working mechanisms of PC-materials [1], [3]. However, much less is known however about the liquid state of these materials despite its prominent role for both amorphization and re-crystallization. Indeed, amorphization is achieved by quenching the liquid, while the fast re-crystallization of amorphous regions takes place above the glass-transition temperature, suggesting that it might proceed through the under-cooled liquid state. Therefore an in-depth knowledge of the structure of the liquid state improves our understanding of both the amorphization and the re-crystallization mechanisms.

Many-ternary Te-based alloys were studied in the liquid state by neutron scattering on the 7C2 diffractometer. The structure of the liquid was shown to depend primarily on the average number of electron per atom.

Using the ratio between the heights of the first two peaks of the total scattering function S(q), two classes of liquids were defined (Figure 2).

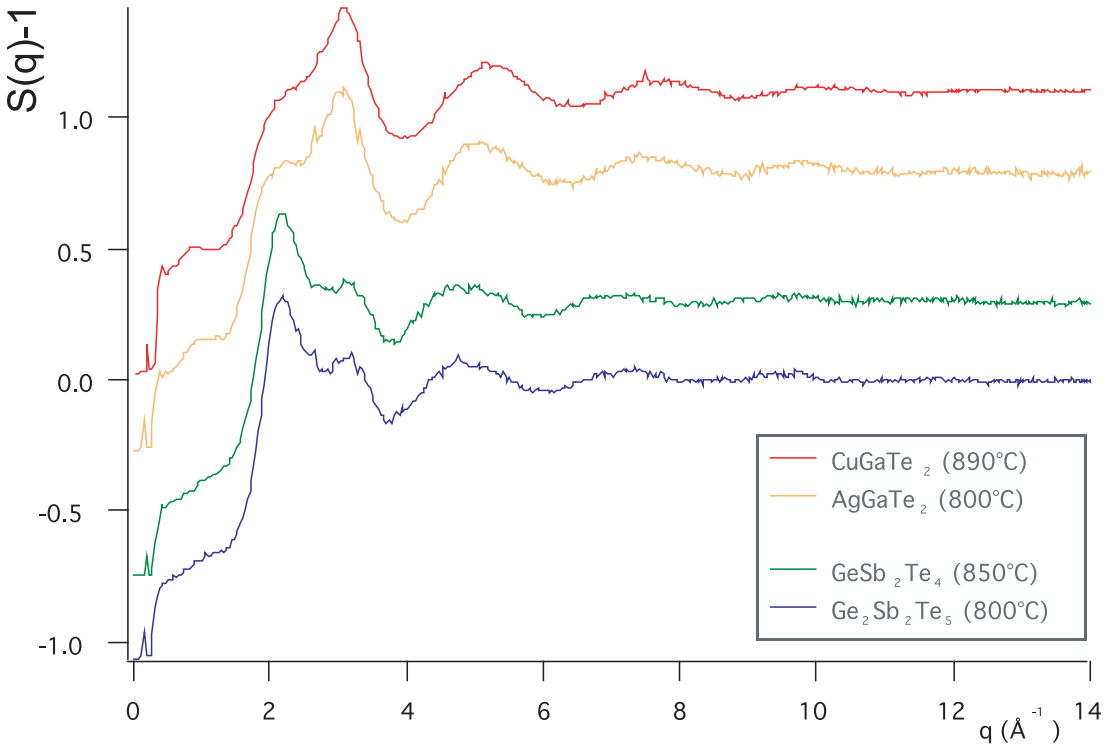

Figure 2: Structure factor of alloys with e/a>4.5 (upper part) and e/a<4.5 (lower part).

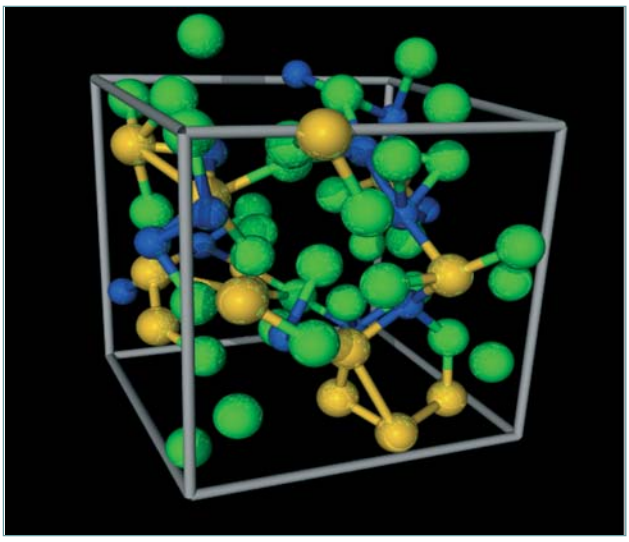

Figure 3: A snapshot of the liquid $Ge_2Sb_2Te_5$ liquid alloy

In the first class with a low number of electrons per atoms ($N_{e/a}$ < 4.5), the structure of the liquid is tetrahedral-like similarly to the solid and the contrast in electrical/optical properties is not sufficient to qualify the material for PC availability. On the contrary, the second class of materials with a higher number of electrons per atoms ($N_{e/a}$ > 4.5) has an octahedral-like local structure and possesses a PC capability.

The local structure of these complex amorphous or liquid materials is largely under discussion ([2], [3], [4]). It cannot be directly extracted from the neutron data only, and other investigations are needed. In parallel to the experimental analyses, computer simulations of the liquid structure are been performed (ab initio molecular dynamics). From these *ab initio* MD experiments, that compare well to the experimental data in the case of $Ge_2Sb_2Te_5$, a detailed analysis of the local order will be made (Figure 3).

It is clear that finding generic features that qualify suitable PC-materials requires a fundamental understanding of the parameters that drive the transition between tetrahedral and octahedral environments. The transition region (around 4.5 electron/atom) will be more closely investigated, as well as the effect of the atomic radii for a given electron/atom ratio.

[1] G.-F. Zhou, Mat. Sci. and Eng. A **304-306**, 3 (2001).

[2] A. Kolobov, P. Fons, A. Frenkel, A. Ankudinov, J. Tominaga, and T. Uruga, Nature Materials **3**, 703 (2004).

[3] W. Welnic, A. Pamungkas, R. Detemple, C. Steimer, S. Blügel, and M. Wuttig, Nature Materials **5**, 56 (2006).

[4] A.V. Kolobov, J. Haines, A. Pradel, M. Ribes, P. Fons, J. Tominaga, Y. Katayama, T. Hammouda and T. Uruga, PRL **97**, 035701 (2006)