

# Early first principles study of $Ga_4Sb_6Te_3$ phase-change material: Liquid and amorphous

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In the few last years, scientists extensively studied phase-change material (PCM) for data storage applications. The  $Ge_2Sb_2Te_5$  (GST) is the material actually used in the DVD's and phase change RAM's. Despite the success of the GST ternary system as a benchmark of phase-change materials, This component suffers from many undesirable properties, namely the relatively low crystallization temperature and activation energy, limiting its data-retention capability, and a high melting temperature [2-6]. Therefore, the discovery of alternative materials is one of the current priorities. In this context, a new PCM raised as a good candidat: The alloy  $Ga_4Sb_6Te_3$  (GaST). This material shows a fast crystallization speed, very high crystallization temperature, ( $T_x$ ), and a high electrical contrast [1].

Extensive first principles molecular dynamics (FPMD) simulations have been performed on the  $Ga_4Sb_6Te_3$  system by using the Car-Parrinello method. We adopted a generalized gradient approximation (GGA) for the exchange and correlation part of the total energy. In particular, the BLYP was used since a recent study [7] showed that BLYP leads to better agreement with experimental structural properties than PBE in case of liquid and amorphous  $Ge_2Sb_2Te_5$ . A norm conserving pseudopotentials are used for the core-valence interactions. Notice that the pseudo potentials of Gallium atom includes the non linear core-corrections. The wave functions are expanded in plane waves basis set at the gamma point of the super cell, with a cutoff energy of 60 Ry. A temperature control is implemented for both ionic and fictitious electronic degrees of freedom by using the Nosé-Hoover thermostats.

Starting from a disordered  $GeSe_2$  amorphous configuration, a 117 atom system was generated and randomized for 40 picoseconds at  $T=2000K$ . The liquid phase was obtained by relaxing the model at  $T=900K$  for 20 ps. The density of the liquid phase at  $T=900 K$  was adjusted by releasing the internal pressure. Further NPT run served to check the density stability. The amorphous phase was obtained by melt-quenching the liquid during 100 ps. Finally the amorphous density was adjusted at 0 K followed by data collection for 20 ps at  $T=300K$ . Figure 1 provides a snapshot of the amorphous structure.

In figure 2 we present the different partials pair distribution functions (PDF) at the liquid and the amorphous state at  $T=900K$  and  $T=300K$  respectively. The different partials PDF show weaker features at  $T=900 K$  indicating a reduced order. At  $T=300 K$  the peaks are sharper and much higher. Additional peaks grow up in the short and long range order region. The first peak in the  $g_{GaGa}(r)$  moves from 2.70 Å at  $T=900 K$  to 2.55Å at  $T=300 K$ . The first minimum

position moves also toward low  $r$  values leading to a reduction in the partial coordination number  $n_{GaGa}$  and to a reduction in the fraction of the homopolar bonds. The second peaks in the  $g_{GaGa}(r)$  moves at higher  $r$  values indicating that a Ga atom can find another Ga as second nearest neighbor. The  $g_{GaSb}(r)$  and  $g_{GaTe}(r)$  features higher first peak at  $2.77 \text{ \AA}$  at  $T=300 \text{ K}$  than  $T=900 \text{ K}$ . This is associated to the increase of the structural organization with the quench. Also two peaks appears at  $4.25 \text{ \AA}$  and  $6.69 \text{ \AA}$ , corresponding to the second and third neighbors shells.

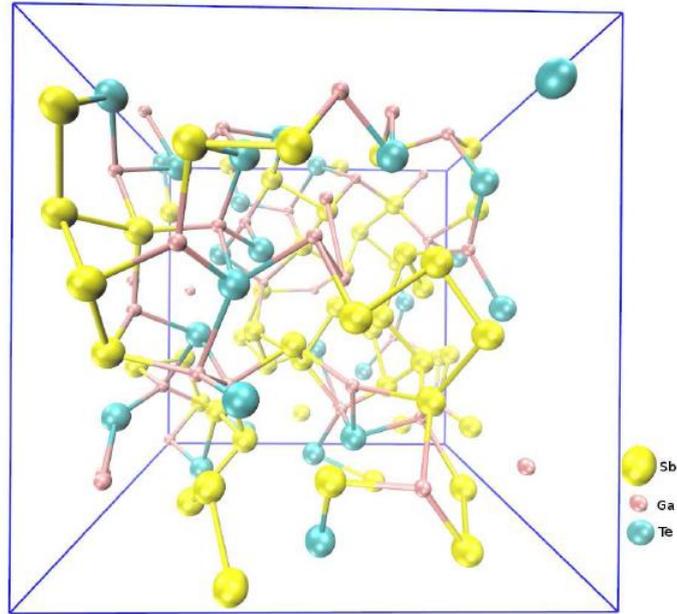


Figure 1: Snapshot of the amorphous  $Ga_4Sb_6Te_3$  at 300K.

Overall, it appears that Ga atoms have most likely Sb and Te atoms as first neighbor, Ga and Sb as second neighbor, while no special preference in regard to the chemical order is found for the third neighbor

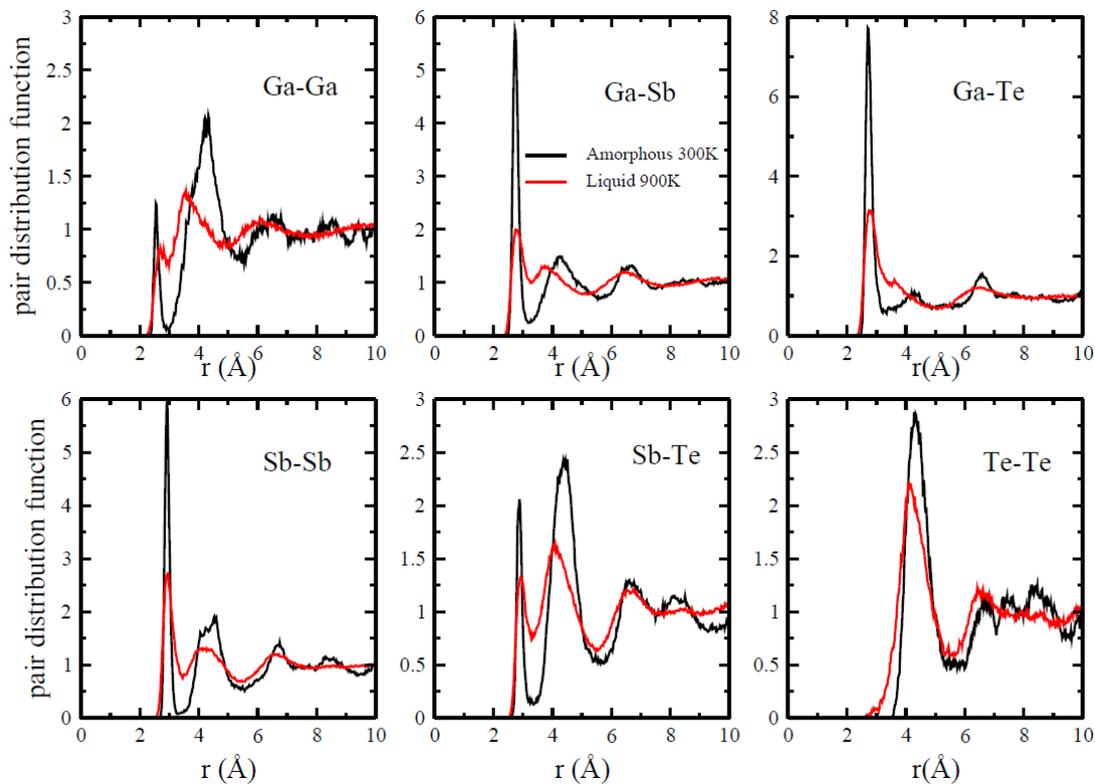


Figure 2: The partials pair distribution functions.

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