

Local order, dynamics and stability of C and N doped phase change materials.

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Doping Chalcogenide Phase Change Materials, such as $\text{Ge}_2\text{Sb}_2\text{Te}_5$ and GeTe used in non-volatile phase change memories, was shown to improve the stability of the amorphous phase and to strongly increase the crystallization temperature. We combined total X-ray scattering experiments [1], Fourier Transform InfraRed (FTIR) spectroscopy and ab initio Molecular Dynamics simulations to address the stabilization of the amorphous phase of GeTe doped with Carbon or Nitrogen. The comparison between the simulation and experimental results allows in depth understanding of the role of dopants. They deeply modify the structure of the amorphous phase by introducing tetrahedral units centered on C or N, triangular environments and short C chains in C-doped GeTe , NGe_3 pyramids and N_2 molecules in N-doped GeTe . One major difference between N and C doping is the fact that C can form short bonds with Te, although in smaller proportion than C-Ge, while short N-Te bonds are absent in N-doped GeTe . The inclusion of C or N leads to an increase in high frequency vibrational modes, to a reduction of the density of floppy vibrational modes that drive the crystallization and to an increase of the rigidity. This stabilization mechanism could apply more generally to various GST materials as well as to other iono-covalent glasses.

[1] G.E. Ghezzi, J.Y.Raty, S. Maitrejean, A. Roule, E. Elkaim and F. Hippert, Appl. Phys. Lett. **99** (2011) 151906.