

Ab-initio study of the structural and vibrational properties of amorphous phase change materials: Sb₂Te₃, GeTe and InGeTe₂

S. Caravati^{1,2}, E. Spreafico², R. Mazzarello¹, M. Parrinello¹ and M. Bernasconi²

¹ Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich, USI Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

² Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi 53, I-20125, Milano, Italy

Based on ab-initio molecular dynamics simulations, we generated models of amorphous Sb₂Te₃, GeTe and InGeTe₂ of interest for applications as phase change materials in electronic data storage. Sb and Te atoms are in a defective octahedral-like geometry similar to that found in the most studied Ge₂Sb₂Te₅ (GST) compound [1,2]. Coexistence of defective octahedral sites with tetrahedral sites for In and Ge are found in InGeTe₂ and GeTe. The calculated Raman spectrum of GeTe is in very good agreement with experimental data [3] and contains the signatures of all the peculiar local structures of the amorphous phase, namely tetrahedral Ge and defective octahedral sites for a fraction of Ge (mostly 4-coordinated) and for all Te (mostly 3-coordinated) atoms. In particular, the spectrum above 190 cm⁻¹ is dominated by tetrahedral structures, while the most prominent peaks around 120 and 165 cm⁻¹ are mainly due to vibrations of atoms in defective octahedral sites. Finally, the peak around 75 cm⁻¹ which dominates the spectrum in HV scattering geometry, is mostly due to vibrational modes involving 3-coordinated Te atoms. Amorphous Sb₂Te₃ displays a larger concentration of nanosized cavities with respect to a-GST and a-GeTe which corroborates the previously proposed [2] correlation between the concentration and size of cavities and the experimental crystallization speed. InGeTe₂, proposed as a candidate material for good data retention [4], also displays a very high density of cavities which suggests that, in spite of the higher crystallization temperature (T_c), its crystallization speed at T_c might be as high as in GeSbTe alloys.

[1] S. Caravati, M. Bernasconi, T. D. Kuehne, M. Krack, and M. Parrinello, Appl. Phys. Lett. 91, 171906 (2007); J. Phys. Cond. Matt. 21, 255501 (2009); Phys. Rev. Lett. 102, 205502 (2009).

[2] J. Akola and R. O. Jones, Phys. Rev. B 76, 235201 (2007).

[3] K. S. Andrikopoulos, S. N. Yannopoulos, A. V. Kolobov, P. Fons, and J. Tominaga, J. Phys. Chem. Sol. 68, 1074 (2007).

[4] T. Morikawa et al, IEEE Electron Devices Meeting, IEDM 2007, 307-310 (2007).