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Effect of carbon and nitrogen doping on the structure of amorphous GeTe phase change material[1] JEAN-YVES RATY, Physics Department B5, University of Liege, 4000 Sart-Tilman Belgium, GIADA GHEZZI, SYLVAIN MAITREJEAN, PIERRE NOÉ, ANNE ROULE, CEA-Leti, Minatec, 17 rue des Martyrs, 38054 Grenoble, France, CHRISTOPHE BICHARA, CINaM-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, France, FRANÇOISE HIPPERT, LMPG-Grenoble, Minatec 3, Parvis L. Néel, 38016 Grenoble, France — Carbon and Nitrogen-doped GeTe are promising materials for use in phase change memories since the addition of C or N increases the stability of the amorphous phase. By combining ab initio molecular dynamics and X-ray scattering experiments, we show that carbon deeply modifies the structure of the amorphous phase through long carbon chains, tetrahedral and triangular units centred on carbon. A clear signature of these units is the appearance of an additional interatomic distance around 3.3 A in the pair correlation function. Besides, the first Ge-Ge and Ge-Te distances are almost not affected by doping. The implications for the vibrational and thermal properties are finally discussed.

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