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Mechanism of GeSbTe phase change materials: an ab initio molecular dynamics study[1] JEAN-YVES RATY, CÉLINE OTJACQUES, JEAN-PIERRE GASPARD, University of Liege, Belgium, CHRISTOPHE BICHARA, CRMCN , University Aix-Marseille, France — Among phase change materials, Ge2Sb2Te5 (225) is one of the most successfully used in applications. Accepted models are based on EXAFS spectra and suppose a complete reorganization of bonds during amorphization, with Ge changing from sixfold to tetrahedral coordination. We perform ab initio MD simulations of the (225), (124) and (415) liquid alloys. We show that the crystalline, liquid and amorphous structure of these systems are similar, with very little sp3 hybridization around Ge atoms and a majority of p-sigma bonds. Using a set of quenched liquid configurations we reproduce the EXAFS measurements on the (225) composition and explain how the static Debye Waller factor due to the vacancies in the crystal phase leads to a cancellation of individual neighbors contribution to the EXAFS signal while in the amorphous, a larger coherence occurs, enhancing the EXAFS signal. The computed electrical conductivities of the three phases (cubic solid, liquid and amorphous) prove to be very different, accordingly with the experiment.

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