

Abstract Submitted
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Temperature induced density anomaly in Te rich liquid Germanium Tellurides : p versus sp³ bonding ?¹ CHRISTOPHE BICHARA, CNRS -CRMCN University Aix-Marseille, France, MARK JOHNSON, Institut Laue Langevin, Grenoble, France, JEAN-YVES RATY, University of Liege, Belgium — The density anomaly of liquid Ge_{0.15}Te_{0.85} measured between 633K and 733K is investigated with ab initio Molecular Dynamics calculations at four temperatures and at the corresponding experimental densities. For box sizes ranging from 56 to 112 atoms, an 8 k-points sampling of the Brillouin zone is necessary to obtain reliable results. Contrary to other Ge chalcogenides, no sp³ hybridization of the Ge bonding is observed. As a consequence the negative thermal expansion of the liquid is not related to a tetrahedral bonding as in the case of water or silica. We show that it results from the symmetry recovery of the local environment of Ge atoms that is distorted at low temperature by a Peierls-like mechanism acting in the liquid state in the same way as in the parent solid phases.

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