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First Principles Study of structural characteristics and phase change mechanism of Ge-Sb-Te based materials HANJIN PARK, CHEOL-WOON KIM, HYUNG-JUNE LEE, HOSIN SONG, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 130-701, Korea — Using *ab initio* density functional theory, we investigate the structural properties and their phase transition mechanism of the crystalline and amorphous phases of Ge-Sb-Te (GST) based phase change materials, which would be utilized for phase change random access memory. Among various stochiometries of GST, we focus on compositions along the $(GeTe)_n(Sb_2Te_3)_m$ pseudo-binary line, denoted simply by (n, m) with integer n and m. We explore various GST materials corresponding (n, m) sets including (1,0), (0,1), (1,1), (2,1) and (1,2) by modeling their both phases. Especially, their amorphous phases can be constructed based on experimental data available or molecular dynamics (MD) simulations performing melt-quench processes. To understand the phase transition mechanism, we evaluate their coordination numbers, radial distribution functions, and angle distribution functions, which enables us to identify the characteristic local geometry representing each phase. We further investigate the thermal properties of various phases by evaluating their phonon densities of states obtained by Fourier-transforming the velocity autocorrelation functions calculated directly from our MD simulation.

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