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Ab Initio Study of Structural Stability and Phase Transition Properties of Phase Transition Material : GeTe HANJIN PARK, CHEOL-WOON KIM, YOUNG-KYUN KWON, Department of Physics and Research Institude for Basic Sciences, Kyung Hee University, Seoul, Korea — Using ab initio density functional calculations, we investigate the structural and electronic properties of the ordered crystalline and disordered amorphous phases of a GeTe material, which would be used for phase change random access memory. With suitable pseudopotentials selected for respective elements, we first explore the equilibrium configurations and electronic properties of their crystalline phases. Different amorphous phases are, then, modeled by performing molecular dynamics simulations, which are composed of various stages including thermal equilibrations, a high-temperature pre-melting process with a low gravimetric density, and a quenching process to room temperature. To identify the local structures in amorphous phases, we evaluate their radial distribution functions (RDFs) and order parameters (OPs). Our calculated OPs and RDFs are analyzed and compared to EXAFS data available. Finally, we estimate energy barriers not only between crystalline and one of amorphous phases, but also between different amorphous phases to explore their structural stability, using nudged elastic band method.

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