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Atomistic origin of doping-enhanced ultrafast crystallization in Ag-doped $Ge_2Sb_2Te_5$ BINAY PRASAI, GANG CHEN, DAVID DRABOLD, Ohio University — We have applied ab-initio molecular dynamics (AIMD) simulations to directly simulate the effects of Ag-doping on the phase change properties of Ge2Sb2Te5. The short range order is preserved, whereas a slight improvement in the chemical order is observed. A slight decrease in the fraction of tetrahedral Ge (sp3 bonding) is reflected in the reduction of the optical band gap and in the increased dielectric constant. Simulations of the amorphous to crystalline phase change cycle revealed the enhanced crystallization speed in Ag0.5Ge2Sb2Te5 as compared to Ge2Sb2Te5. Moreover, the smaller density difference and the larger energy difference between the two phases of Ag0.5Ge2Sb2Te5 (compared to Ge2Sb2Te5) suggest a smaller residual stress in devices due to phase transition and improved thermal stability for Ag0.5Ge2Sb2Te5. The potential viability of this material suggests the need for a wide exploration of alternative phase change memory materials.

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