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Molecular dynamics study on volume dependence of atomic and electronic structure in amorphous $Ge_2Sb_2Te_5$ JINO IM, CHANGWON PARK, JISOON IHM, Department of Physics and Astronomy, Seoul National University, EUNAE CHO, SEUNGWU HAN, Department of Physics, Ewha Womans University — In order to understand the confinement effect of the phase-change memory cell consisting of $Ge_2Sb_2Te_5$, we carry out first-principles molecular dynamics calculations with the simulation volume equal to or larger than the crystalline volume. The amorphous structures are obtained by rapidly quenching the liquid phase of $Ge_2Sb_2Te_5$. It is found that the energy gap increases monotonically with the simulation volume. Furthermore, the density of defect levels in the energy gap is reduced in the simulation using the large cell volume. The resistance drift of the phase-change memory cell is explained on the basis of the simulation results.

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