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Local structure and Phase transition of $(\text{GeTe})_n(\text{Sb}_2\text{Te}_3)_m$ pseudo-binary system for the phase-change memory JINO IM, JAE-HYEON EOM, JISOON IHM, Department of Physics and Astronomy, Seoul National University, Seoul, Korea — A theoretical investigation on the local structure and phase transition between the crystalline and the amorphous phase of $(\text{GeTe})_n(\text{Sb}_2\text{Te}_3)_m$ pseudo-binary system(GST) for the phase-change memory is presented. Based on the study of the coordination number for the amorphous phase of GST, the local structure of the amorphous phase of the GST is shown to be composed of the stibnite-like building block for the Sb₂Te₃ and chain-like building block for the GeTe. The phase transition between the crystalline and the amorphous phase of GST is explained by relative repositioning of these building blocks. Density functional total energy minimization calculations show that the crystallization energy and the volume change in transition also agree with experimental data.

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