

Abstract Submitted  
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**Insights into the structure of the stable and meta-stable  $(\text{GeTe})_m(\text{Sb}_2\text{Te}_3)_n$  compounds** JUAREZ L.F. DA SILVA, ARON WALSH, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA, HOSUN LEE, Dept. of Applied Physics, Kyung Hee University, Suwon 446-701, South Korea — Phase-change materials such as  $(\text{GeTe})_m(\text{Sb}_2\text{Te}_3)_n$  (GST) have been considered as one of the most natural candidates for the development of non-volatile memory devices, however, there is no common consensus on the structure of those compounds. Using first-principles calculations, we identify the mechanisms that lead to the lowest energy structures for the crystalline GST compounds, namely, strain energy release by the formation of superlattice structures along of the hexagonal [0001] direction and by maximizing the number of Te atoms surrounded by three Ge and three Sb atoms (3Ge-Te-3Sb rule), and Peierls-type bond dimerization. The intrinsic vacancies form ordered planes perpendicular to the stacking direction in both phases, which separate the GST building blocks. The 3Ge-Te-3Sb rule leads to the intermixing of Ge and Sb atoms in the (0001) planes for  $\text{Ge}_3\text{Sb}_2\text{Te}_6$  and  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ , while only single atomic species in the (0001) planes satisfy this rule for the  $\text{GeSb}_2\text{Te}_4$  and  $\text{GeSb}_4\text{Te}_7$  compositions.

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