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The local structural differences in amorphous Ge-Sb-Te alloys

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Abstract

Chalcogenide alloys in pseudobinary line between Sb_2Te_3 and GeTe are extensively utilied in phase change memories for optical and electronic contrast between crystalline and amorphous phases. Different from the crystalline structure, the understanding of amorphous structures is still insuffient due to disorder and distortion. By employing first-principle molecular dynamics simulations and atomistic cluster alignment analysis, the short-range orders and the associated distortions of amorphous Sb_2Te_3, $Ge_1Sb_2Te_4$, $Ge_2Sb_2Te_5$, $Ge_3Sb_2Te_6$ and GeTe are investigated to explore the origin of nature difference. The results reveal that Ge-Ge and Sb-Sb bonds present a notable competitive mechanism with GeTe content. The GeTe content has a great influence on Ge- and Te-centered short-range orders but little influence on the structures of Sb-centered clusters, especially for the octahedral sites and unidentified structures. The tetrahedrons in Ge-centered clusters of each alloy show a close proportion, but the fraction of tetrahedrons in total clusters increases with the increasing GeTe content due to the increase in the ratio of Ge atom. As for the distortions of clusters, the distorted tetrahedrons in $Ge_2Sb_2Te_5$ are closest to the standard tetrahedron, the Peierls distortion of Ge-centered 6-fold octahedron reduces