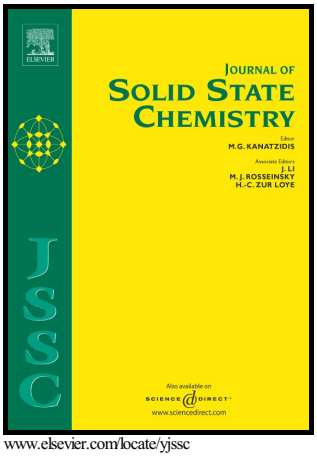
Effect of gradual ordering of Ge/Sb atoms on chemical bonding: a proposed mechanism for the formation of crystalline $Ge_2Sb_2Te_5$

Janpreet Singh, Gurinder Singh, Aman Kaura, S.K. Tripathi



www.elsevier.com/locate/yjssc

PII: S0022-4596(18)30036-7
DOI: https://doi.org/10.1016/j.jssc.2018.01.021
Reference: YJSSC20097

To appear in: *Journal of Solid State Chemistry*

Received date: 29 September 2017
Revised date: 19 December 2017
Accepted date: 22 January 2018

Cite this article as: Janpreet Singh, Gurinder Singh, Aman Kaura and S.K. Tripathi, Effect of gradual ordering of Ge/Sb atoms on chemical bonding: a proposed mechanism for the formation of crystalline $Ge_2Sb_2Te_5$, *Journal of Solid State Chemistry,* https://doi.org/10.1016/j.jssc.2018.01.021

Effect of gradual ordering of Ge/Sb atoms on chemical bonding: a proposed mechanism for the formation of crystalline $Ge_2Sb_2Te_5$

Janpreet Singh[1], Gurinder Singh[2], Aman Kaura[2] and S.K. Tripathi[1*]

[1]*Department of Physics, Centre of Advanced Study in Physics, Panjab University, Chandigarh, 160014, India*

[2]*Department of UIET, Panjab University SSG Regional Centre Hoshiarpur, Panjab, India*

**Electronic mail: surya@pu.ac.in; surya_tr@yahoo.com*

Abstract

Using first principle calculations, we study the atomic arrangement and bonding mechanism in the crystalline phase of $Ge_2Sb_2Te_5$ (GST). It is found that the stability of GST depends on the gradual ordering of Ge/Sb atoms. The configurations with different concentration of Ge/Sb in layers have been analyzed by the partial density of state, electron localization function and Bader charge distribution. The s and p-states of Ge atom alter with different stacking configurations but there is no change in Sb and Te atom states. Our findings show that the bonding between Ge-Te is not only responsible for the stability of GST alloy but can also predict which composition can show generic features of phase change material. As the number of Ge atoms near to vacancy layer decreases, Ge donates more charge. A growth model has been proposed for the formation of crystalline phase which justifies the structure models proposed in the literature.

Keywords: Gradual ordering; Chemical bonding; Density functional theory; Electron localization function; Bader charge analysis; Crystal growth model.

Graphical Abstract

This paper shows the effect of gradual ordering of Ge/Sb atoms on the chemical bonding viz. partial density of states, electron localization function and Bader charge. A possible growth model for the formation of crystalline $Ge_2Sb_2Te_5$ has been proposed based on the calculated binding energy order using density functional theory with PBE functional.