Thermoelectric properties of two stacking sequences of crystalline GST-225

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abstract

Pseudobinary GeTe-Sb_2Te_3 compounds are widely used as phase-change optical materials for DVD-RAM.[3] $Ge_2Sb_2Te_5$ (GST-225) is used for this propose but the stacking sequence of the stable crystal structure is motive of debate. Pseudobinary compounds there are claimed to be good thermoelectric materials due the large number of intrinsic structural vacancies.[4] Thermoelectric properties for two proposed stacking sequences of GST-225 are computed using DFT[5, 6] and Boltzmann transport equation in the constant relaxation time approximation. After phonon calculations, no dynamic instabilities were found in the Irreducible Brillouin Zone for either of the proposed stacking sequences. One of the stacking sequences shows semiconductor-like density of states (DOS) with a computed gap of 190 meV unlike the other stacking sequence which has a metallic-like DOS. Thermoelectric properties calculation reveals that semiconductor-like structure has the highest value of Seebeck coefficient (SC)(at 650K $S_{xx} \approx 100$ against 45μV/K of the metallic-like). Our theoretical results of SC are in good agreement with experimental data.

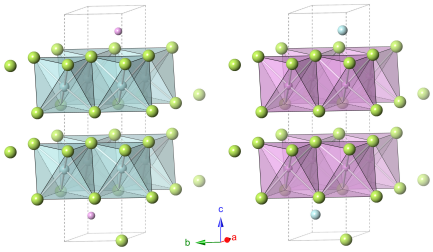

Figure 1: *The two proposed stacking sequences for GST-225. The stacking proposed by Kooi and De Hosson is Te-Ge-Te-Sb-Te-Te-Sb-Te-Ge-[1] (left) and the one proposed by Petrov et al.[2] derives from the previous one by the exchange of Sb and Ge layers (right). Green, violet and light blue represent Te, Ge and Sb atoms respectively.*

References

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