Supplementary Information

For

Optic phonons and anisotropic thermal conductivity in hexagonal $Ge_2Sb_2Te_5$

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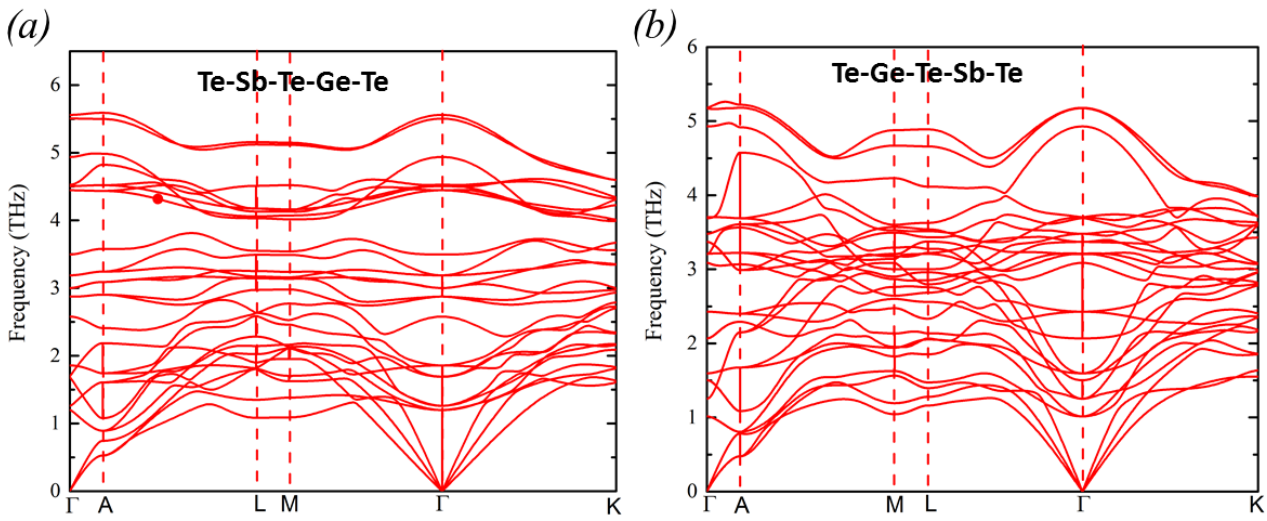

Figure S1: Phonon dispersion of h-GST for (a) Te-Sb-Te-Ge-Te and (b) Te-Ge-Te-Sb-Te stacking as given by Mantsunga[1,2] and Kooi[3], respectively.

Joint density of state (JDOS): JDOS was calculated based on the harmonic force constants using the following expressions:

$$N_2^{(1)} = \frac{1}{N}\sum_{\lambda'\lambda''} \Delta(-q+q'+q'')(n_{\lambda'} - n_{\lambda''})[\delta(\omega+\omega_{\lambda'}-\omega_{\lambda''}) - \delta(\omega-\omega_{\lambda'}+\omega_{\lambda''})]$$

$$N_2^{(2)} = \frac{1}{N}\sum_{\lambda'\lambda''} \Delta(-q+q'+q'')(n_{\lambda'} + n_{\lambda''} + 1)\delta(\omega-\omega_{\lambda'}-\omega_{\lambda''})$$

With $N_2^{(1)}$ and $N_2^{(2)}$ representing the number of scattering processes of $\delta(\omega-\omega_{\lambda_1}-\omega_{\lambda_2})$ or $\delta(\omega+\omega_{\lambda_1}-\omega_{\lambda_2})$ kind, respectively. Here, we are considering scattering of phonon λ with λ'

and λ'' with wave vectors $q, q' \, and \, q''$ and frequencies$\omega, \omega_{\lambda_1} \, and \, \omega_{\lambda_2}$, respectively. $n_{\lambda'} \, and \, n_{\lambda''}$ are the Bose distribution function for phonons $q' \, and \, q''$ calculated at T=300K.

References

[1] T. Matsunaga, R. Kojima, N. Yamada, K. Kifune, Y. Kubota, and M. Takata, Appl Phys Lett **90**, 161919 (2007).

[2] T. Matsunaga and N. Yamada, Phys Rev B **69**, 104111 (2004).

[3] B. J. Kooi and J. T. M. De Hosson, J Appl Phys **92**, 3584 (2002).