Determination of thermal properties of diamond using cellular monte carlo

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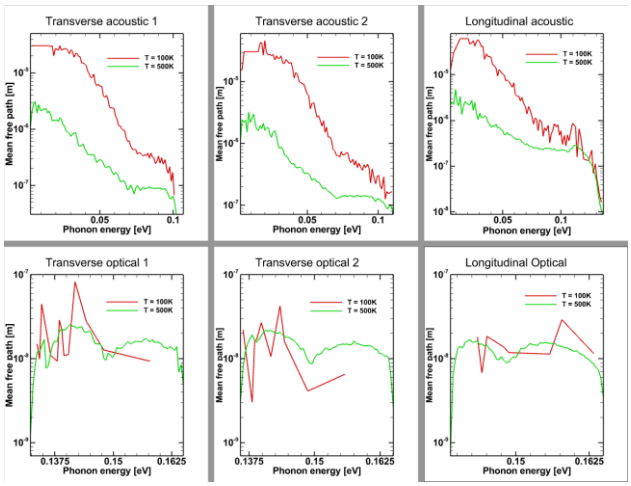
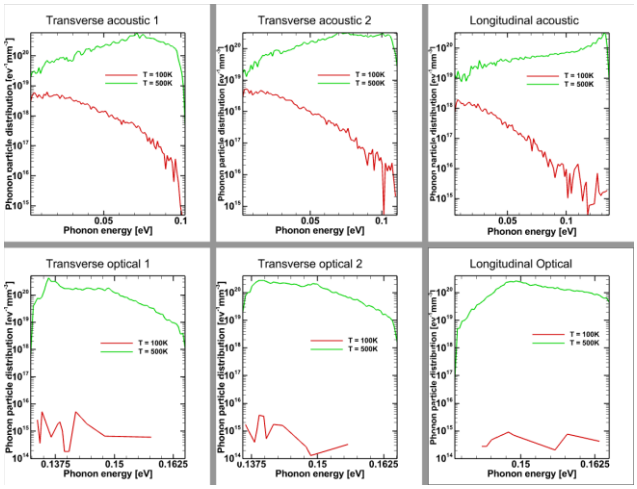
1. Introduction

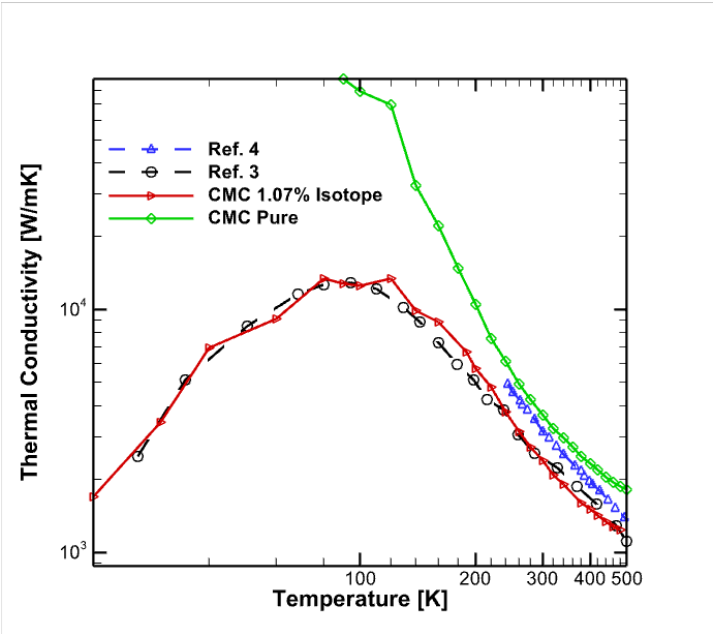
I In this paper we evaluate the thermal properties of diamond by determination of phonon transport properties in bulk crystal. We solve the full non-linear Peierls-Boltzmann transport equation using Cellular Monte Carlo [1,2] method to obtain phonon occupation numbers while they scatter through three-particle interaction in momentum space and with isotopes and impurities present in the diamond crystal. We report the simulation results from 60K to 500K for diamond doped with isotope C_{13} (1.07%) and for pure diamond from 100K – 500K. Our results are in excellent agreement with the experimental values. Longitudinal acoustic mode appears to be the prime carrier of thermal current at 500K.



Phonon mean free path



Phonon particle distribution



Bulk thermal conductivity of natural and pure diamond

Reference:

[1] Saraniti, Marco, and Stephen M. Goodnick. "Hybrid fullband cellular automaton/Monte Carlo approach for fast simulation of charge transport in semiconductors." IEEE Transactions on Electron Devices 47, no. 10 (2000): 1909-1916.

[2] Sabatti, Flavio FM, Stephen M. Goodnick, and Marco Saraniti. "Simulation of phonon transport in semiconductors using a population-dependent many-body cellular monte carlo approach." Journal of Heat Transfer 139, no. 3 (2017).

[3] Berman, R., P. R. W. Hudson, and M. Martinez. "Nitrogen in diamond: evidence from thermal conductivity." Journal of Physics C: Solid State Physics 8, no. 21 (1975): L430.

[4] Onn, 2_DG, A. Witek, Y. Z. Qiu, T. R. Anthony, and W. F. Banholzer. "Some aspects of the thermal conductivity of isotopically enriched diamond single crystals." Physical review letters 68, no. 18 (1992): 2806.