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Thermal Expansion in Graphene and Graphane: Role of Anharmonic and Harmonic Effects ARUNIMA SINGH, RICHARD G. HENNIG, Department of Materials Science and Engineering, Cornell University — As the practical application of graphene nears realization, knowledge of effects of temperature on mechanical properties of graphene becomes important. In this study we use empirical potentials and density-functional perturbation theory (DFPT) to determine the thermal expansion of free-standing graphene, graphene on substrates, and its hydrogenated derivative graphane. Comparisons of MD simulations with calculations using the quasi- harmonic approximation using an empirical potential show that anharmonic effects are negligible at temperatures below 2200K. In contrast to the DFPT calculations using the quasi-harmonic approximation, MD results show that free-standing graphene has a positive thermal expansion coefficient above 600K. For graphene on a substrate our DFPT results agree with those of Jiang et. al [1] and show that the substrate suppresses the negative thermal expansion coefficient with increasing strength of the substrate- graphene interaction. We also investigate the thermal expansion of the thermodynamically stable conformers of graphane using DFPT.

[1] J. W. Jiang, J. S. Wang, B. Li, Phys. Rev. B 80, 205429 (2009).

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