A Group Theoretic Approach to Nonlinear and Gradient Elastic Terms for Graphene and Carbon Nanotubes

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Abstract

Nonlinear and gradient corrections to the elastic theory of graphene and carbon nanotubes are important for determining the thermal conductivity, mechanical properties under large deformations, dissipation in nanotube oscillators and other mechanical properties. By applying group theory, we can systematically and efficiently work out all nonlinear elastic terms that can appear in a Ginzburg-Landau formulation of the elastic free energy in terms of the material displacement gradient tensor. Graphene serves as a perfect example material, having an interesting hexagonal symmetry and being a material in which nonlinear elastic terms are important. This approach allows us to demonstrate the usual cubic corrections. Additionally, we find higher order strain corrections which correspond to bending and rolling the graphene sheet, as well as gradient terms which are important for describing the long wavelength phonon dispersion. We will enumerate the most important contributions to the free energy, and measure the corresponding elastic constants with simulation.