Scaling behaviour of in-plane elastic properties of graphene

J. H. Los, A. Fasolino and M. I. Katsnelson

Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

In this work study the scaling behaviour of in-plane elastic properties of graphene, such as the bulk modulus. While for a 'normal' 3D crystal, system size dependence of the bulk modulus is basically unthinkable, here we show by performing Monte Carlo simulations that the bulk modulus of graphene obeys a power law $B \propto L^{-\nu}$ with L the linear size of the (square) system and ν ' 0.3, roughly in agreement with predictions from membrane theory within the self-consistent screening approximation. Not covered by membrane theory, our results also reveal a very strong anisotropy with an unusual negative cubic term and, consequently, an unusual equation of state which is poorly described by the Murnaghan equation. Here we present an alternative expression for the equation state, able to describe the simulation data accurately, which can be expected to be of general applicability to 2D solids embedded in 3D space. With this expression we are able to explain the recent, experimental observation of a quite strong increase of the elastic modulus by a factor 2 or more of graphene under only very weak tensile strain as small as 0.5 %.