Prediction of Mechanical properties of wrinkled and defective graphene via molecular mechanics study

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Wrinkling is a natural phenomena in suspended graphene, thus it is expected to have substantial effect on behavior of mechanical properties upon introduction of straining. We have obtained the mechanical properties such as elastic modulus, stress-strain relation of wrinkled graphene under three different strain directions (i.e. transverse, longitudinal direction, and biaxial strain) with molecular dynamics simulation. Furthermore, effects of vacancy defects have been studied under strained condition of wrinkled graphene. It is found that the large out-of-plane deformation and the low stiffness of graphene are observed due to defects, which are modeled to follow regular and irregular positions depending on concentration. We found that the inclusion of wrinkled region to mechanical property calculation offers 2nd and 3rd elastic modulus in good agreement with reference values, and the vacancy defects largely affect small strain region, thus the stiffness of wrinkled graphene.