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A New Molecular Structural Mechanics Model for the Flexural Analysis of Monolayer Graphene

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Summary

Based on molecular mechanics, a new structural mechanics model, a 2-D frame composed of equivalent anisotropic beams and flexible connections, is proposed for the simulation of the static and dynamic flexural behavior of monolayer graphene. The equivalent beam representing the C-C bond in the new molecular structural mechanics (MSM) model has two salient features compared with other MSM models proposed for the analysis of carbon nanotubes: one is that the flexible connections at the beam ends are used to account for the bond-angle variations between the C-C bonds; and the other is that there are two principal bending rigidities used, respectively, for the in-plane bending energy associated with bond angle variations and the inversion energy to characterize the different behaviors of the i?3-bond and i??-bond in the graphene lattice. The mechanical properties of the equivalent beam representing the C-C bond in the graphene lattice are evaluated from the molecular mechanics. The in-plane mechanical properties as well static and vibrational flexural behaviors of monolayer graphene are analyzed using the proposed new MSM model coupled with ANSYS. The simulation results show that the 2-D flexibly connected frame model of the new MSM model proposed in this paper gives improved predictions of the in-plane Young's moduli, Poisson ratios and flexural rigidities of monolayer graphene than other MSM models. The present study also indicates that the modeling of bond angle variation is very important in the mechanical behavior simulations of graphene lattice. For example, the present new MSM model in which a monolayer graphene is modeled as flexibly connected planar lattice predicts very good results of Poisson ratios of graphene, but on the other hand the original MSM model in which a monolayer graphene is modeled as rigidly connected planar lattice yields much smaller Poisson ratios although this structural mechanics model is able to predict a quite good longitudinal deformation, The present study also shows that monolayer graphene sheet is kind of an anisotropic material since both the in-plane elastic properties and the flexural rigidities of monolayer graphene are chirality dependent.