A Modified Molecular Structure Mechanics Method for Analysis of Graphene

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The molecular structure mechanics method has been one of the most effective ways to investigate the mechanical properties of graphene. However, graphene is considered as the equivalent space frame composed of rigid connections, which is not consistent with the real deformation. In this paper, in order to improve the method, a modified molecular structure mechanics method was developed, in which the semi-rigid connections are used to model the bond angle variations between the C-C bonds in graphene. The simulated results show that the equivalent space frame model with semi-rigid connections for graphene proposed in the article is simple, efficient and accurate. Though the present computational model of the semi-rigid connected space frame is only applied to characterize graphene, it has more potential applications in the static and dynamic analyses of other nanomaterials.

Keywords: Graphene, molecular structure mechanics, semi-rigid connections, mechanical properties