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ABSTRACT

In recent years, shape design of graphene sheets (GSs) by introducing topological defects for enhancing their mechanical behaviors has attracted the attention of scholars. In the present work, we propose a consistent methodology for optimal shape design of GSs using a combination of the molecular mechanics (MM) method, the non-parametric shape optimization method, the phase field crystal (PFC) method, Voronoi tessellation, and molecular dynamics (MD) simulation to maximize their fundamental frequencies. At first, we model GSs as continuum frame models using a link between the MM method and continuum mechanics. Then, we carry out optimal shape design of GSs in fundamental frequency maximization problem based on a developed shape optimization method for frames. However, the obtained optimal shapes of GSs only consisting of hexagonal carbon rings are unstable that do not satisfy the principle of least action, so we relocate carbon atoms on the optimal shapes by introducing topological defects using the PFC method and Voronoi tessellation. At last, we perform the structural relaxation through MD simulation to determine the final optimal shapes of GSs. We design two examples of GSs and the optimal results show that the fundamental frequencies of GSs can be significantly enhanced according to the optimal shape design methodology.

Keywords: Graphene sheets; Natural frequency; Optimal shape design; Topological defects.