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Shape Optimum Design of Graphene Sheets

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Abstract

Graphene sheet (GS) is a monolayer of carbon atoms arranged in a honeycomb lattice and is the strongest material ever measured and the thinnest material ever synthesized in the universe. Due to its unique mechanical, structural and electronic properties, GS is supposed to be a base material for nanoelectromechanical systems (NEMS), given that lightness and stiffness are the essential characteristics sought in NEMS for sensing applications. In this study, shape optimum design of GS is carried out to improve its stiffness for these applications. At first, we model C-C bond as an equivalent continuum beam by means of molecular mechanics (MM) method. So that GS can be adopted as a continuum frame structure. Then, we optimize the shape of the atomistic finite element model based on a free-form optimization method for frame structures. In the optimization process, we use the compliance as objective function and minimize it under the volume constraint. Each equivalent continuum beam is assumed to vary in the off-axis direction to the centroidal axis and we derive the shape gradient function for determination of the optimal design velocity field based on the free-form optimization method. Using the derived optimal design velocity field, the shape optimum design of GS can be carried out without shape parametrization. The numerical results show that, using the proposed shape optimization method, the compliance of GS can be significantly reduced that would be helpful for designing GS used in NEMS.

Keywords: Compliance; Free-form; Graphene sheets; Molecular mechanics; Shape optimum design.