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A plate model for multilayer graphene sheets and its finite element implementation via corotational formulation

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Abstract

An equivalent continuum model for multilayer graphene sheets (MLGSs) and its plate model are developed to analyze the deformation behavior of MLGSs. Hyperelastic material models are introduced for the MLGS continuum model by examining the atomistic structures of MLGSs and obtaining their mechanical properties by means of molecular statics simulations. The MLGS plate model, a structural model for MLGSs, is developed by applying kinematics assumptions to the MLGS continuum model subjected to infinitesimal deformation. Finite element methods (FEM) with the corotational formulation are adopted to analyze the mechanical behavior of MLGSs under small-strain deformation and large rotation conditions. The MLGS plate element passes several basic numerical tests, including patch tests, eigenvalue analyses, and geometrically nonlinear benchmark problems. Finally, the deflections of a plane-strain cantilever and spherical indentations are analyzed by the proposed MLGS plate element and molecular dynamics (MD) simulations. These results show that the MLGS plate element properly represents the deformation behaviors of MLGSs from the atomic scale to the macroscopic continuum scale.

Keywords: Graphene, plate model, corotational formulation, molecular dynamics simulations

1. Introduction

Multilayer graphene sheets (MLGSs) a two-dimensional material [1] composed of graphene layers, have distinct optical [2], electronical [3], thermal [4, 5] and mechanical [6] properties. Owing to their superior features, there are various applications of MLGSs, such as