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Atomistic–continuum coupled model for nonlinear analysis of double layer graphene sheets using hierarchical multi-scale simulation

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Graphene sheet have attracted considerable attention since it was discovered in 2004. This has been because of its exceptional features. The mechanical and electrical properties of graphene have been perceived to be closely coupled with deformation morphologies. Therefore, alterations in these properties of graphene by controlling the deformation morphologies have been considered very important. In this study, a multi-scale hierarchical molecular mechanic (MM)–finite element (FE) coupling methods are proposed to illustrate the influence of strain on mechanical properties of double-layer graphene sheets (DLGS) in large deformation. The Airebo interatomic potential is employed to describe the interaction between bonded atoms in single layer graphene sheet (SLGS) and non-bonded atoms in graphene layers. Nonlinear elastic parameters of DLGS in large deformation under uniaxial and biaxial strains along armchair and zigzag directions are obtained by computing second-order derivative of strain energy density with respect to deformation criterions. To bridge between atomistic and continuum level, the mechanical characteristics are investigated by molecular mechanic (MM) calculations at the atomistic level and transferred to the continuum level directly by functions of strains. Furthermore, comparing the numerical results of the present multi-scale method with MM simulation results discloses the suggested technique produce promising results with acceptable amounts of error in large deformation. In order to capture quantities of strain energy density conforming to empirical potentials at atomistic scale, a rectangular computational cell with fixed boundary conditions is used as a representative volume element (RVE) of a DLGS. Elastic constants graphs are illustrated as a function of green strains. The elastic tensor components utilized in FEM analysis and results were compared with a full atomic model.

Biography

Mohsen Motezaker is pursuing his MSc in Structural Engineering at Sharif University of Technology, Iran. His MSc thesis entitled “Multi-scale simulation of carbon nanotubes using coupled atomistic-continuum modeling”. His research will propose a single layer graphene sheet as the primary substance of carbon nanotubes. This research is designed for the analysis of deformation effect of the graphene sheet on mechanical properties of CNTs in order to consider that as a curved shell. He has previously worked with Dr. Reza Kolahchi on “The nonlinear buckling response of embedded piezoelectric cylindrical shell” and “Buckling analysis and smart control of SLGS”. His research interest includes “Computational nano-mechanics and large deformation analysis”.

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