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Effect of radial stretch on vibration characteristics of single-layered circular graphene sheets GUNJAN PAHLANI, Mechanical Engineering, Indian Institute of Tech Hyderabad, DEEPTI VERMA, CEMS, University of Minnesota, SHAKTI GUPTA, Mechanical Engineering, Indian Institute of Tech Kanpur
— Vibrations of single-layered circular graphene sheets are studied using molecular mechanics (MM) simulations. Interactions between bonded and non-bonded atoms are prescribed using MM3 potential. Frequencies of different modes of vibration are computed from the eigenvalues and eigen vectors of mass weighted Hessian of the system. This study is performed on graphene sheets of various diameters. A linear continuum membrane model for predicting vibrational frequencies is studied using finite element (FE) method. Frequencies for several modes computed from continuum and molecular model matched well for moderate values of radial stretch, however, with increased stretch those deviated from each other significantly. In particular for higher values of stretch the MM simulations predict considerably lower values of frequencies compared to that found from FE simulations. Also, at higher values of stretch the frequency vs. stretch curve obtained from MM simulations showed a hardening behavior which could not be captured by the linear continuum model. We have also found a similar behavior in two-layered graphene sheets using MM simulations.

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