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Molecular Dynamics Simulation of Free Vibration of Graphene Sheets

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Abstract : TThis paper considers vibration of single-layered graphene sheets using molecular dynamics (MD) and nonlocal elasticity theory. Based on the MD simulations, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), an open source software, is used to obtain fundamental frequencies. On the other hand, governing equations are derived using nonlocal elasticity and first order shear deformation theory (FSDT) and solved using generalized differential quadrature method (GDQ). The small-scale effect is applied in governing equations of motion by nonlocal parameter. The effect of different side lengths, boundary conditions and nonlocal parameter are inspected for aforementioned methods. Results are obtained from MD simulations is compared with those of the nonlocal elasticity theory to calculate appropriate values for the nonlocal parameter. The nonlocal parameter value is suggested for graphene sheets with various boundary conditions. Furthermore, it is shown that the nonlocal elasticity approach using classical plate theory (CLPT) assumptions overestimates the natural frequencies.

Keywords : graphene sheets, molecular dynamics simulations, fundamental frequencies, nonlocal elasticity theory, nonlocal parameter
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