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Molecular Dynamics Analysis on Impact Behaviour of Carbon Nanotubes and Graphene Sheets

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Abstract : Impact behavior of striker on graphene sheet and carbon nanotube is investigated based on molecular dynamics (MD) simulations. A MD simulation is conducted to obtain the maximum dynamic deflections of a square and rectangular single-layered graphene sheets (SLGSs) with various values of side-length and striker parameter. Effect of (i) chirality, (ii) graphene side-length and nanotube length, (iii) striker mass on the maximum dynamic deflections of graphene and nanotube are investigated. The effect of different types of boundary condition on the maximum dynamic deflections is studied for zigzag and armchair SWCNTs with various aspect ratios (Length/Diameter).

Keywords: impact, molecular dynamic, graphene, spring mass

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