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The Study on Mechanical Properties of Graphene Using Molecular Mechanics

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Abstract : The elastic properties and fracture of two-dimensional graphene were calculated purely from the atomic bonding (stretching and bending) based on molecular mechanics method. Considering the representative unit cell of graphene under various loading conditions, the deformations of carbon bonds and the variations of the interlayer distance could be realized numerically under the geometry constraints and minimum energy assumption. In elastic region, it was found that graphene was in-plane isotropic. Meanwhile, the in-plane deformation of the representative unit cell is not uniform along armchair direction due to the discrete and non-uniform distributions of the atoms. The fracture of graphene could be predicted using fracture criteria based on the critical bond length, over which the bond would break. It was noticed that the fracture behavior were directional dependent, which was consistent with molecular dynamics simulation results.

Keywords : energy minimization, fracture, graphene, molecular mechanics
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