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Computational analysis of the effect of Boron and Nitrogen dopants on the mechanical properties of graphene with single vacancy defects

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ABSTRACT

Graphene has a wide range of applications in nanocomposites, nano transistors, nano sensors, nano electronics and Micro/Nano electromechanical systems (M/NEMS) due to its unique properties. In M/NEMS applications such as graphene resonator, piezoresistive sensors, strain sensors, resonant sensors, force and charge sensors, piezoelectric actuators, etc. both the electrical and mechanical properties of graphene have equal importance. The dopant atoms boron and nitrogen are proved to be efficient in improving the semiconducting and electrical properties of graphene and thus its performance in nanoelectronics and nanodevices may be enhanced. Also having valency and atomic number closer to carbon, makes them easier substitutional dopants. But these dopant atoms also disrupt the ideal carbon atoms sp2 hybridization in graphene that can deteriorate its extraordinary mechanical properties. Along with these dopant atoms, there are inherent unavoidable defects generated in graphene that may majorly affect its mechanical properties. Hence, a good comprehension of the defects and dopants induced in graphene would be beneficial for further enhancement in graphene-based nano engineering. Therefore, in the present research, Molecular dynamics simulations were performed to study the effects of dopanatoms with varying doping and defect concentrations, on the mechanical properties of a monolayer graphene. The effects of defect and dopants on the mechanical properties of graphene sheet, including, fracture strength, fracture strain and Young's modulus were analysed. The defect considered was single vacancy and the dopants considered were Boron (B) and Nitrogen (N) atoms. The defect concentrations from 0 to 2% with the doping concentrations from 0 to 5% were considered in the study. The molecular modelling of graphene was done using VMD (Visual Molecular Dynamics). The defects and dopants in the graphene were added using Avogadro. The uniaxial tensile test simulations on graphene models were performed using LAMMPS (Large- scale Atomic/Molecular Massively Parallel Simulator). The desired mechanical properties were extracted from the simulation results and visualized using MATLAB and OVITO (Open Visualization Tool). Substantial decrease was observed in the values of mechanical properties of graphene sheets with the rise in defect concentration. Higher fracture strength results were observed in N-doped graphene models, whereas the B-doped graphene gives higher fracture strain results. The Young's modulus of graphene shows linear rise after reduction, with increase in N doping concentration, whereas the value falls or remains stable after reduction, with increase in B doping concentration. The doping concentrations of each dopant element that shows maximum values of the mechanical properties of graphene at each defect concentrations were identified. The obtained MD simulation results are beneficial in the selection of optimal doping concentration, affordable defect concentration and suitable dopant atom for the development of graphene-based M/NEMS.

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