Effect of Horizontal and Vertical Strains on Graphenes with Vacancies

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With molecular dynamics method, physical strengths of defective graphenes have been explicitly investigated by applying two types of strains depending on the direction of tension: horizontal and vertical. The horizontal directions for straining are categorized to be longitudinal, transverse, and biaxial. Vertically, the indentation is only considered. Also, it is important to notice the difference between periodic and non-periodic graphenes when the simulation work is performed for accurate property-analysis on the bulk phase and the independent. Thus, both systems are considered in this work. We applied those tensions to the systems with different number densities of defects to obtain their strengths by calculating strain energy and estimating second and third elastic modulus. We found that the strength of defective graphene depends on the amount of defects and the orders of them, which are analyzed by the radial distribution function applied to defect sites.