The Mechanical Properties of Graphene with Different Defects

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Graphene, formed by one layer of hexagonally patterned carbon atoms, has attracted great attention in various application areas because of its extraordinary mechanical, physical and chemical properties. The mechanical properties of perfect graphene have been investigated intensively and have already been widely accepted. However, most of the graphenes have defects in fact, such as Thrower–Stone–Wales defect, the change of grain boundary of different orientation. How the defects affecting the mechanical property of graphene is still an open question. Our studies mainly focus on the impact of these various defects on mechanical properties of graphene, and its failure mechanism. The deformation behavior and the mechanical properties of graphene with different defects are investigated by using molecular dynamics simulation. Furthermore, molecular dynamic simulations are performed to demonstrate the mechanical properties of hybrid graphene and boron nitrogen sheet with different concentration. The results reveal that the mechanical properties of the hybrid graphene and boron nitrogen sheet should be considered carefully in evaluating its performance.

Keywords: Graphene; Grain boundary; Molecular dynamics simulations; Mechanical properties.