Mechanical properties of twisted bilayer graphene

Qiang Cao

The Institute of Technological Sciences, Wuhan University, Wuhan 430072, China

Corresponding author: caoqiang@whu.edu.cn

Abstract

As a special two-dimensional material with single-atom thickness, graphene possesses extraordinary properties and fascinating applications. Mechanical properties of graphene are part of the hottest topics in graphene research. Most of the mechanical properties of graphene such as Young's modulus, Poisson's ratio, strength and fracture toughness have been studied sufficiently since 2004. Here we reported something new in the mechanical properties of graphene discovered by molecular dynamics simulations. Our simulations indicated that graphene can enhance the critical yield strength, hardness and elastic modulus of the graphene/Fe composite to different degrees with the change of the number of graphene layers, which makes it an ideal material in the reinforcement of metal-matrix composites. When stacking two sheets of graphene that are twisted relative to each other by a certain angle, the so called twisted bilayer graphene (tBLG) is formed, which exhibits many new properties. The tensile simulation for tBLGs with different twist angles along the in-plane direction showed that their elastic properties is dominated by the orientation of graphene layers and present slight difference with traditional bilayer graphene (BLG). The compression simulation along the transverse direction showed that the intrinsic strength of tBLG increases with the increasing twist angle within certain limits. This revealed the potential application of tBLG in ballistic protection. Further simulation proved that tBLG with certain twist angle exhibits higher ballistic resistance capacity than BLG. Such improvement in ballistic resistance capacity is possibly caused by the slower but isotropic energy dispersion process during ballistic impact. This means that tBLG is a more potential ballistic protection material than BLG.

Keywords: Graphene; Twisted bilayer graphene; mechanical properties; molecular dynamic simulation