INTRINSIC STRENGTH AND FAILURE BEHAVIORS OF GRAPHENE GRAIN BOUNDARIES

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In the experimental fabrications of large-scale graphene using chemical vapor deposition method, achieving polycrystalline graphene composed of many single-crystal domains separated by grain boundaries (GBs) is almost inevitable. As one-dimension line defects, GBs can affect many intrinsic properties of graphene. Here, we present a DFT and molecular dynamics study on the mechanical properties of 20 representative graphene GBs. With different arrangements of the pentagonal and heptagonal rings, the grain boundary may remain flat or become inflected up to 72° For the flat GBs, the intrinsic tensile strength decreases linearly with the formation energy with a maximum value of 93 GPa, close to that of a perfect graphene. The intrinsic tensile strength of the inflected GBs is found to generally decrease with increasing inflection angle. Stone-Wales transformation is identified as the major failure mechanism of graphene GBs at high temperatures, whereas the initial fracture site can be either on the boundary line or inside the domain. These theoretical results constitute a useful picture of the grain boundary effect on the mechanical properties of polycrystalline graphene.

[1] Junfeng Zhang, Jijun Zhao and Jianping Lu, ACS Nano, **6**, 2704 (2012).