Ideal Strength of Doped Graphene

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A recent nanoindentation experiment, which has shown that graphene is the strongest two dimensional meterial, reports that the intrinsic strength of graphene is 42 N/m at the nominal equibiaxial breaking strain of 0.225 [1]. This was followed by a theoretical calculation [2] showing the quite smaller breaking strain of 0.15 than the measured value. It is unusual since materials under strain typically fail before they reach the ideal strength. We have considered electronic doping as a possible external factor to reduce the gap between the experiment and theory [3].

While the mechanical distortions change the electronic properties of graphene significantly, the effects of electronic manipulation on its mechanical properties have not been well known. Using first-principles calculation methods, we show that, when graphene expands isotropically under equibiaxial strain, both the electron and hole doping can improve its ideal strength and enhance the critical breaking strain dramatically. We have further found that, contrary to the isotropic expansions, under uniaxial strain, the electron doping decreases the ideal strength as well as critical strain of graphene while the hole doping increases both. Strengthening or weakening of graphene upon doping is associated with the modification of Fermi surfaces, electron-phonon interaction, Kohn anomaly and the change of electronic band structures. We will discuss the distinct failure mechanisms which depend on type of strains related with the different doping-induced mechanical stabilities and instabilities.

References

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