Conversion of multilayer graphene into ultrathin diamond-like material

황대연, Kester Wong, 곽상규†
울산과학기술원
(skkwak@unist.ac.kr†)

We studied how multilayer graphene can undergo transformation into sp^3 structure by using density functional theory (DFT) method and predicted diamond-like properties in multilayered sp^3 structures at varying thickness. Herein, hydrogenation of multilayer graphene at the both sides of surface induce a sp^2 to sp^3 transition and as a result, a diamond-like structure can be obtained. Surface hydrogenation reduces the transition barrier due to the low stability of hydrogen passivated graphene layer caused by unpaired electrons. Electronical and mechanical properties of sp^3 multilayer graphene were calculated by varying the number of carbon layers and the stacking orientation of the sp^3 structure. The sp^3 structure exhibited various electronical and mechanical properties indicative of a diamond material, except that the electrons of conduction band were mainly distributed at the hydrogenated surface. This is due to the top and bottom surface stabilization through termination with hydrogen. By extrapolating the band gap and Young's modulus of our structures under consideration, we successfully identified the thinnest possible sp^3 structures that exhibit diamond-like properties.