Thematic area of the work: Nanoscale physics

Electronic properties of tensile-stressed impure graphene

I.Yu. Sagalianov[1], T.M. Radchenko[2], Yu.I. Prylutskyy[1], V.A. Tatarenko[2]

[1]*Taras Shevchenko National University of Kyiv,*
64 Volodymyrska Street, UA-03022 Kyiv-22, Ukraine

[2]*G.V. Kurdyumov Institute for Metal Physics, NAS of Ukraine*
36 Academician Vernadsky Boulevard, UA-03680 Kyiv-03142, Ukraine
E-mail: tarad@imp.kiev.ua

Currently, mass-production of graphene-based switch devices is obstructed by the band gap absence. To solve this problem (engineering a band gap in graphene) many efforts are currently applying in various ways: cutting graphene into nanoribbons (nanomeshes), applying perpendicular magnetic field to bilayer graphene, surface adsorption or/and introducing specific defects, utilization of strain, etc. Graphene is the strongest material ever tested with an intrinsic tensile strength of ~130 GPa, Young's modulus of ~1 TPa and even increases with the density of defects. Graphene sheet can sustain reversible (elastic) deformations up to about ≈25–27%. That is why the strain yields an interesting possibility to tune the properties of graphene and thus opens a new field called "straintronics".

Over the past five years, dozens of papers dealing with influence of different types of strain on electronic properties of (mainly defect-free) graphene have been published. Among already obtained (theoretical) results, there are questionable and discussable ones. The presence of disagreements is not surprising inasmuch as two reasons. First, "straintronics" only opens its evolution. Second, in overwhelming majority of theoretical and computational studies of the strained graphene, the size of graphene computational domains are mostly limited to periodic supercells and localized fragments containing a relatively small number (usually some hundreds) of atoms (sites). These restrictions are caused by the commonly used first-principles density-functional calculations requiring high computational capabilities.

Our study deals with the band gap in uniaxially tensile-stressed graphene doped by spatially ordered impurity (ad)atoms, when the scattering process is rather inefficient and gives rise to quasi-ballistic transport more than to quasi-diffusive one, i.e. at an electronic transport with low scattering. We study peculiarities of the strain-dependent bad-gap opening if any, namely, its width depending on concentration of adatoms, type of adsorbing sites, and stress. Conditions and restrictions, at which the strain and dopant (ad)atomic ordering act as competitive or mutually complementary factors, are identified.