The hexagon molecular motive as main factor for the failure of chemically modified graphene

Shaymardanova L.Kh.*, Sheka E.F., Popova N.A.

Peoples' Friendship University of Russia, 117198 Moscow, Russia
**e-mail: landy.nur@gmail.com*

Recently the response of a nanographene sheet to external stresses has been considered in terms of a mechanochemical reaction [1-3]. As shown, a high stiffness of the graphene body is connected with that of the benzenoid unit. The anisotropy of the unit mechanical behavior in combination with different packing of the units either normally or parallel to the body C-C bond chains forms the ground for the structure-sensitive mechanism of the mechanical behavior of the object that drastically depends on the deformation modes. The mechanical behavior of graphene under *zg* and *ach* deformation modes is similar to that of a tricotage when either the sheet rupture has both commenced and completed by the rupture of a single stitch row (*ach* mode) or the rupture of one stitch is 'tugging at thread' the other stitches that are replaced by still elongated one-atom chain of carbon atoms (*zg* mode). For the first time, the approach makes allowance for tracing deformation-stimulated change in the chemical reactivity of both nanographene sheet as a whole and its individual atoms in terms of total and partial numbers of effectively unpaired electrons.

The current paper presents a comparative study of mechanical properties of a set of molecules involving hexametyl (HXM) and hexamethylene (HXMe) benzene, HXM cyclohexane, HXM hexafluoro cyclohexane, and HXM cyclobornitrid (HXM B_3N_3) that constitute the main hexagon patterns of pristine and chemically modified graphene as well as its bornitrid analogue under uniaxial tension. HXM and HXMe framing of the molecules makes the molecule hexagon motive alike to that of the related graphenium bodies. Cyclohexanes in both cases correspond to chair-like conformers.

As follows from the study, both the Young moduli and their gradual lowering when going from HXM benzene to HXM hexafluoro cyclohexane and HXM cyclobornitrid are well consistent with experimental data related to graphene and both graphane $(CH)_n$, graphene fluoride $(CF)_n$ as well as to bornitrid analogue $(B_3N_3)_n$ thus confirming the hexagon pattern responsibility for both mechanical characteristics of graphenium bodies and mechanical anisotropy of their properties.

[1] E.F. Sheka, N.A. Popova, V.A. Popova, E.A. Nikitina, L.Kh. Shaymardanova. arXiv:1005.0796 [cond- mat_mess-hall], 2010.

[2] E.F. Sheka, N.A. Popova, V.A. Popova, E.A. Nikitina, L.Kh. Shaymardanova. *J. Exp. Theor. Phys.* **139**(4) (2011).

[3] E.F. Sheka, N.A. Popova, V.A. Popova, E.A. Nikitina, L.Kh. Shaymardanova. *J. Mol. Mod.* DOI: 10.1007/s00894-010-0816-3, 2011.