Effect of chemical modification on tricotage-like deformation of graphene

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The response of a nanographene sheet to external stresses can be successfully considered in terms of mechanochemical reaction [1-3]. The quantum chemical realization of the approach is based on the coordinate-of-reaction concept for introducing a mechanochemical internal coordinate (MIC) that specifies a deformational mode. The related force of response is calculated as the energy gradient along the MIC, while the atomic configuration is optimized over all of the other coordinates under the MIC constant-pitch elongation. The approach has been applied first to the benzene molecule and (5, 5) nanographene [1-3]. In the current study the response to uniaxial tension has been considered concerning hexamethyl cyclohexane (HMCH) molecule and (5, 5) nanographane sheet.

The quantum-mechanochemical-reaction-coordinate approach has disclosed atomically matched peculiarities that accompany the deformation-failure-rupture process occurred in the bodies. A high stiffness of both graphene and graphane bodies is provided by the related hexagon units. The two units are characterized by anisotropy in the microscopic behavior under elongation along a MIC when the MIC is oriented either along (*zg*) or normally (*ach*) to the C-C bonds chain. The unit feature in combination with different configuration of the units packing with respect to the body C-C bond chains forms the ground for the structure-sensitive mechanical behavior that is drastically different for *zg* and *ach* deformation modes. The *zg* deformation mode is particularly manifested with the formation of one-atom chains. Hydrogenation of graphene drastically influences both behavior and numerical characteristics of the body making tricotage-like pattern of the graphane failure less pronounced.

[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.