Electronic and elastic properties of diamond films with nanometer thickness

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The graphene as two-dimensional material has attracted attention from the scientific community long before experimental fabrication. The first theoretical study of graphene is dated 1946, when the remarkable band structure of "Dirac cones" has been studied. First experimental observation of free standing graphene in 2004 [1] initiated the comprehensive study of this material.

Hydrogenation of graphene enlarges its potential application in nanoelectronics. Regular adsorption of hydrogen atoms changes graphene electronic structure and opens the band gap depending upon the distance between hydrogen regions. Total hydrogenation of graphene changes the nature of electronic states due to changing of sp^2 hybridization of C-C bonds to sp^3 one and opens the dielectric band gap. Such two-dimensional insulator was called as graphane. Graphane is an offspring of graphene along with graphene nanoribbons and carbon nanotubes. The other type of carbon bonding opens a new way for developing of two-dimensional carbon based materials.

Graphane is the first member in a series of sp^3 bonded diamond films with nanometer thickness (or diamanes) consist of a number of adjusted $\langle 111 \rangle$ oriented layers which display unique physical properties. The consequent study of graphene, graphane and proposed diamanes can be considered as bottom-up nanotechnological approach opposite to ordinary top-down paradigm. The main goal of this work is to study diamane physical properties. We consider diamanes with different thickness; we investigate their stability and compare them with known data for sp^3-hybridized hydrocarbon clusters. We study the elastic properties of the structures and obtain phonon dispersion, wave velocities and elastic constants. Finally we discuss possible ways to synthesize the structures.

[1] K.S. Novoselov, D. Jiang, F. Schedin, T.J. Booth, V.V. Khotkevich, S,V, Morozov, A.K. Geim, *Proc. Natl. Acad. Sci. USA* **102**, 10451 (2005).