

Theoretical investigation of semiconducting, mechanically stiff diamondfilms of nanometer thickness

Pavel B. Sorokin, Alexander G. Kvashnin, Leonid A. Chernozatonskii and Boris I. Yakobson
Technological Institute of Superhard and Novel Carbon Materials, Moscow, Russian Federation
Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 4 Kosygin st., Moscow, Russian Federation
Rice University, Houston, Texas, USA

pbsorokin@tisnum.ru

Functionalization of graphene enlarges its potential application in nanoelectronics. Total hydrogenation leads to transformation of semimetallic graphene to insulating graphane. Graphene can be considered as the first member in a series of sp^3 bonded diamond films with nanometer thickness consist of a number of adjusted oriented layers with unique physical properties

We investigated electronic properties of the films with different crystallographic orientation of the surface and found that in distinction from graphane diamond films display semiconductor properties with effective mass close to bulk diamond. All hydrogenated films display direct band gap with nonlinear quantum confinement response upon the thickness whereas films with clean surface display both metallic and semiconducting electronic structure depending upon the surface orientation

We studied the elastic properties of the structures. We found that such films are stiff but flexible and can be elastically bent out of plane. Values of the elastic constants and the acoustic velocities of hexagonal diamond (lonsdaleite) films are higher than for cubic diamond films with the same thickness. This makes hexagonal diamond films second in stiffness only to the bulk lonsdaleite and graphene (Fig. 1).

Finally we studied the stability of the diamond films with a clean surface and hydrogenated structures of various thicknesses and found the critical size at which a diamond film splits into the multilayered graphene. We investigated the chemically induced phase transition when adsorption of adatoms to graphene leads to the formation of diamond films without the energy barrier. We obtained the phase

diagram (P,T,d) of the 2D carbon films of a d thickness from which the conditions of diamond films formation from the multilayered graphene can be defined.

Figures

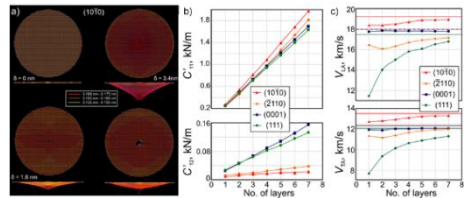


Figure 1: a) the deformation sequence for hexagonal diamond films with (1010) surface: unloaded structure, with indentation depth $\delta=1.6$ nm, $\delta=3.4$ nm (critical strain), and after the failure. The color variation represents the bond lengths, from red (0.168–0.175 nm) to yellow (0.135–0.155 nm); The dependence of the b) elastic constants $11 C'$, $12 C''$ and c) velocities of longitudinal v_{LA} and transverse v_{TA} acoustic waves of the hexagonal diamond films with (1010) (\blacktriangle), (111) (\blacklozenge) and (0001) (\blacksquare) surfaces for different number of layers (different thickness) in comparison with cubic diamond films with (111) surface (\bullet).

References

- [1] A.G. Kvashnin, L.A. Chernozatonskii, B.I. Yakobson, P.B. Sorokin, Nano Letters 14 (2014) 676
- [2] A.G. Kvashnin, P.B. Sorokin, J. Phys. Chem. Lett. 5 (2014) 541