Vacancies influence on elastic properties of graphene and their migration rate under deformation

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Formation and properties of defects, first of all – single vacancies inside sp2 form of carbon (graphite, graphene and carbon nanotubes (CNT)) have been investigated in many works, both experimental and theoretical [1,2,3]. This intereSt is explained by determinative role of such defects during utilization of graphite inside nuclear reactors, junction of CNT under irradiation etc. At that majority of works was deal with electronic, geometrical and magnetic structure of the defects. Investigations of dynamics of vacancies and their influence on elastic properties of sp2 form of carbon, especially under deformations practically absent. So, in this work influence of the vacancies on elastic properties of graphene and their migration rate under deformations are investigated by DFT calculations with help of VASP [4] package.

At that nearly linear negative dependence of graphene Young moduli on vacancies concentration has been detected, see Fig.1. One can see the Young modulus values can be decreased at ~20% when a distance between nearest vacancies is ~12Å. Also potential barrier values for single vacancies jumps between neareSt positions are calculated for different deformations. Using transition state theory the dependence of vacancies migration rate on applied deformation is calculated for different temperatures. It is shown this rate can be changed on ~10 orders of magnitude by using deformation of 5% only.

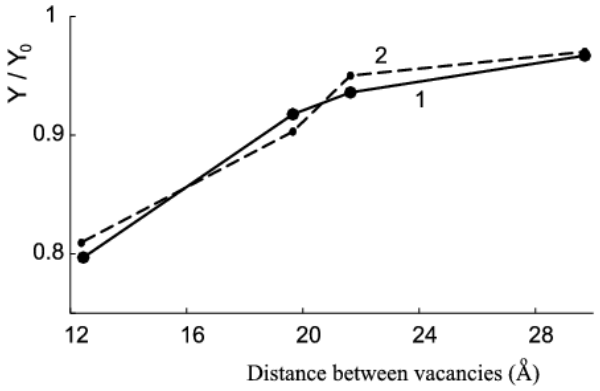

Figure 1. Dependence of ratio of defective graphene Young moduli to moduli of defect-free graphene on distance between neareSt vacancies. Curve 1 correspond on deformation along X axis, 2- along Y axis.

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