

# A hyperboloid structure as a mechanical model of the carbon bond



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## ARTICLE INFO

### Article history:

Received 16 September 2015

Revised 3 May 2016

Available online 18 June 2016

### Keywords:

Mechanics of carbon bond  
Mechanics of nanostructures  
Hyperboloid model  
Structural model  
Molecular mechanics

## ABSTRACT

We present a new mechanical model of interatomic bonds, which can be used to describe the elastic properties of the carbon allotropes, such as graphite, diamond, fullerene, and carbon nanotubes. The interatomic bond is modeled by a hyperboloid–shape truss structure. The elastic characteristics of this bond are determined. Previous known structural models also used elastic elements (beams, trusses) to simulate a carbon bond. However unlike them our model satisfies to the correct ratio of the longitudinal and lateral stiffness, observed from the previous experimental and theoretical results. Parameters of the bond in application for graphene and diamond were determined.

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## 1. Introduction

Mechanical properties of carbon nanostructures have been extensively studied by scientists all over the world since the middle of the twentieth century. The elastic properties of two most common allotropes of carbon: diamond and graphite were experimentally determined in works [McSkimin and Andreatch Jr \(1972\)](#); [McSkimin and Bond \(1957\)](#) and [Blakslee et al. \(1970\)](#), respectively. Due to the unique crystal structure, diamond and lonsdaleite are considered as the most durable of the existing materials. At the same time it was predicted that graphite should also have an outstanding tensile strength in the basal plane, but the plane orthogonal to the base has significantly lower tensile strength ([Blakslee et al., 1970](#); [Bosak et al., 2007](#)). Discovery of such materials as fullerenes ([Kroto et al., 1985](#)), carbon nanotubes ([Iijima et al., 1991](#)), and graphene ([Geim and Novoselov, 2007](#)) at the turn of the present century, warmed up the interest of the scientific community to the properties of carbon and the structures it is capable to form.

A key point in the study of the carbon allotropes and its properties at the micro level is the choice of a model describing the interatomic bonds. The ab initio methods developed in the past decade due to the advances of quantum physics and chemistry are widely used to model carbon nanostructures ([Bichoutskaia et al., 2006](#); [Kudin et al., 2001](#); [Yanovsky et al., 2009](#); [Zhou et al., 2001](#)). Apparently, they are the most precise and predictively valid methods,

but due to the high complexity and high computational costs, they are rarely used to describe even relatively small nanostructures, not to mention the objects of the size of a few micrometers. Various particle dynamics methods to simulate carbon nanostructures were applied in order to decrease the simulation time in comparison to ab initio approaches: molecular dynamics ([Golovnev et al., 2008](#); [Jin and Yuan, 2003](#); [Reddy et al., 2006](#); [Yao et al., 2001](#)) and molecular mechanics ([Korobeynikov et al., 2014](#)). These methods suggest that atoms interact as material points through the empirical interaction potentials. In turn, these potentials are partly based on the quantum mechanical calculations. Such approaches reduce the problem to the solution of the ordinary differential equations at each time step. In addition, they require significantly less computational cost than ab initio methods.

At the same time it was shown ([Berinskii and Krivtsov, 2010](#); [Zhang et al., 2002](#)) that a number of commonly used interaction potentials to simulate the graphene, graphite and diamond bonds ([Allinger et al., 1989](#); [Brenner et al., 2002](#);  [Tersoff, 1988](#)) do not meet the experimentally determined elastic moduli. Furthermore, the empirical interaction potentials depending on the position of a number of particles include a large number of parameters with no clear physical meaning. At the same time they are inferior to the pairwise potentials of the Lennard-Jones or Morse type that depend only on the difference between the position vectors of the interacting particles. However, the classical pairwise potentials do not adequately describe the majority of covalent structures, which include carbon allotropes. Such structures are characterized by a low crystal packing density and oriented interatomic bonds. The use of a pairwise potential leads to the maximizing of a packing density that in turn causes the collapsing of a model. A possible

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solution is to take the rotational degrees of freedom for the carbon atoms into account (Grekova and Zhilin, 2001; Ivanova et al., 2007; Vasiliev et al., 2010) and develop a generalized moment (torque) potentials (Berinskii et al., 2007; Kuzkin and Krivtsov, 2011; Kuzkin and Asonov, 2012; Tovstik and Tovstik, 2012) for simulations. In these works the atoms are assumed to be the solid bodies, not just the material points, and interaction between them is described both by the forces and the torques. It gives the interatomic bond additional lateral stiffness, providing the desired angle between the bonds in the lattice. Torque potentials combine the relative simplicity (they are, in fact, pairwise) and versatility. They independently determine the longitudinal, lateral, torsional and flexural bond rigidity. On the one hand it gives the freedom to choose the parameters of the simulation. On the other hand, if the longitudinal and lateral stiffness can be unambiguously determined from the experimentally measured elastic characteristics, the flexural and torsional bond stiffness depends on the couple-stress tensor components of the crystal lattice, for which to date there is no experimental data. On the macrolevel taking the rotational degrees of freedom into account allows to construct a generalised model of material (Eremeyev et al., 2012; Forest et al., 2000; Maugin and Metrikine, 2010).

The foregoing approaches can be attributed to the discrete methods, meaning that the crystal lattice is considered to be a set of interacting particles. However, there are some other approaches that are closer to the field of the classical mechanics. Such approaches are so-called structural or discrete-continuous methods (Cheng et al., 2009; Goldstein et al., 2008; Kalamkarov et al., 2006). The most straightforward example of the structural method is a covalent bond modeled by the solid deformable rod (Li and Chou, 2003; Tserpes and Papanikos, 2005). The distinction of these methods from the discrete ones consists in that the interatomic bonds are modeled as a deformable body or a construction. Besides the perception simplicity, these approaches have one more important advantage. They can be implemented in standard computing packages based on the finite-element, boundary-element, or finite difference methods. These methods can be considered as the bridges between the parameters of atomistic and continual models of the material. E.g. the classical elastic continual model has to be isotropic in case of graphene (Berinskii and Borodich, 2013a) and therefore has only two independent parameters.

The interatomic bond energy can be specified by a interatomic potential as a function of the distance between the nearest interacting atoms and the angles between the adjacent bonds in the lattice. The parameters of the potentials are chosen based on the elastic properties of the entire lattice. At the same time, the binding energy is equivalent to the energy of the rod deformation that depends on its length and its angular deflection. By comparing the energies one can determine the parameters required for the rod model. In particular, if the Euler-Bernoulli model of the rod is considered, then the parameters are Young's modulus of the bond and its diameter. More complex models can be used, e.g. the Timoshenko beam. However in this case an additional parameter appears namely the Poisson ratio of the rod. Its exact value cannot be determined (Berinskii et al., 2014). The circular section rod model imposes some limitations on the properties of carbon bond, but at the same time it allows to determine not only the longitudinal and transverse, but also the torsional and flexural stiffness using only two parameters. These parameters are necessary to determine the bending stiffness of a crystal lattice of the graphene sheet (Berinskii et al., 2014). Modelling of the graphene layer deformation with regard to the available experimental data shows that the ratio of the lateral bond stiffness  $C_2$  between the carbon atoms to the longitudinal stiffness  $C_1$  is approximately 1/2 (Ivanova et al., 2007). However, the rod bond model at the reasonable parameters

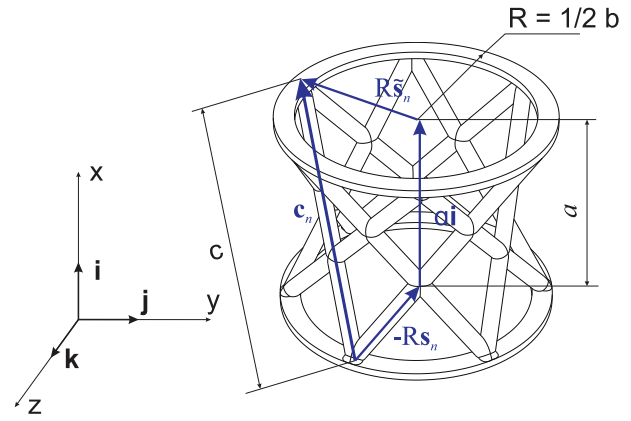


Fig. 1. 3D model of the carbon interatomic bond.

give a much lower value of the flexural rigidity. Thus, the value of 1/2 can only be achieved if the thickness of the rod is close to its length and the material of the rod should have the negative Poisson ratio (Berinskii and Borodich, 2013b). So, an important issue is to find a relatively simple mechanical model that allows for such a ratio of stiffness.

There are other conclusive structural models of the graphene and nanotubes, e.g. (Goldstein et al., 2008; Odegard et al., 2002). However, we have shown earlier (Berinskii and Borodich, 2013b) that they cannot meet the required stiffness ratio.

In this paper, the carbon bond model is built on the symmetry properties of the hyperboloid. These properties allow it to achieve a high ratio of the lateral and longitudinal stiffness, therefore the hyperboloid shapes are widely used in the engineering to create lightweight constructions consisting of straight beams that are known for being able to carry a large load while achieving a low use of raw materials. In particular, the first hyperboloid tower was built by Russian engineer V.G. Shukhov in Nizhny Novgorod (1896) (English, 2005). Being widely demanded in architecture and engineering, such models still haven't found a wide use in micro- and nanomechanics. It appears that the analogy drawn from the macro level will allow to describe correctly the properties of carbon materials at the micro level.

## 2. A hyperboloid carbon model: compression and tension stiffness

We model a carbon bond as a rigid structure, which is constructed as follows. Let us introduce the unit vectors of Cartesian basis  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$ . Here and after the vector and tensor values are denoted by bold letters. Unit vector  $\mathbf{i}$  determines a direction of the bond, unit vectors  $\mathbf{j}$  and  $\mathbf{k}$  determine a plane perpendicular to the bond. Next, consider a cylinder with an axis coinciding with the bond direction, and with the height equal to its length. Bases of the cylinder have a radius of  $R = b/2$ , where  $b$  is a bond width.

Then place a set of  $N$  truss elements with stiffness  $k$  along the generatrices of the cylinder so that they are evenly distributed over the cylinder surface. We then rotate one of the bases of the cylinder around its axis until it makes an angle  $\gamma$ . Then the trusses will rest on the one-sheet hyperboloid surface connecting the two cylinder bases (Figs. 1 and 2). Vectors  $\mathbf{c}_n$  connecting the start and the end point of the truss members of hyperboloid may be represented as

$$\mathbf{c}_n \stackrel{\text{def}}{=} -R\mathbf{s}_n + a\mathbf{i} + R\tilde{\mathbf{s}}_n, \quad (1)$$

where

$$\mathbf{s}_n \stackrel{\text{def}}{=} \mathbf{P}\left(\frac{2n\pi}{N}\mathbf{i}\right) \cdot \mathbf{j}, \quad \tilde{\mathbf{s}}_n \stackrel{\text{def}}{=} \mathbf{P}(\gamma\mathbf{i}) \cdot \mathbf{s}_n; \quad n = 1, 2, \dots, N; \quad (2)$$

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