MODELS OF DIAMOND AND GRAPHENE BASED ON MOMENT AND MULTYBODY INTERACTIONS

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Summary This work is devoted to the mechanical properties of two-atomic crystal lattices such as lattices of graphene, diamond, and silicon. Different approaches of discrete modeling and simulations are used. Presented approaches allow to obtain natural linkage between the discrete and continuum description of the crystalline solids.

Computer simulations are widely used to describe the properties of materials at the micro level. The development of nanotechnology is connected with a great interest to carbon materials with exceptional mechanical properties. These objects include previously unknown allotropic modifications of carbon such as nanotubes, fullerenes, carbon nanofibers, nanodiamonds, graphene and many others. The applications of the mechanical properties of graphene and diamond are very challenging. Therefore the study of these properties is an important and urgent task.

This work is devoted to the mechanical properties of two-atomic crystal lattices such as lattices of graphene, diamond, and silicon. Here we model a graphene layer as an effective 2D continuum having the same properties of symmetry as a real graphene crystal lattice. It is shown that the elastic properties of the linearized model of the effective 2D continuum are isotropic. It is known an isotropic elastic material is an elastic material whose symmetry group does contain proper orthogonal group for a reference configuration and, therefore, the mechanical response of the material exhibits no preferred direction, the property that characterizes material isotropy. The symmetry properties of the stiffness tensor of an elastic continuum are usually studied either by direct consideration of particular cases of symmetry transformations. However the latter approach is rather sophisticated and it is not a trivial task to apply this approach to particular cases of symmetry. Of course, one can write the general expression for re-calculating of the stiffness components in new coordinates and then check if they are the same. However, we believe that it is simpler to follow the general approach for determination of elastic properties of effective continuum models for 3D crystals described by Slawinski [1]. Thus, we consider further the transformation matrices satisfying the symmetry properties of the graphene crystal lattice and this approach is used to describe elastic properties of effective 2D model of graphene.

Different approaches of discrete modeling and simulations are used. One way to model interatomic bonds in graphene is based on the approaches of discrete mechanics. The atoms of carbon in graphene or diamond are modeled by particles with different types of interaction such as force, moment and many-particle interaction. The force interaction is described by central forces between particles such as linear springs or Lennard-Jones potential. It is shown that Odegard model [2] is a particular case of the force interaction model. The moment approach takes moment interactions into account in addition to the force interaction. Every atom of crystal lattice is represented as a solid particle. As a result, the forms of interactions between the particles are more complicated than in case of material points. This way leads to the generalized continuum with rotational degrees of freedom [3]. Finally, the many-particle interaction takes into account the effect of the electronic environment on the diatomic interaction [4]. This way is widely accepted to construct molecular dynamics semi-empirical potentials such as Tersoff-Brenner and MM3 force fields. An approach is proposed that permits calculating the elastic characteristics of crystals by using the interatomic interaction parameters specified as many-particle potentials. The many-particle interaction is given in the general form obtained in the framework of linear elastic deformation. It is shown that in quadratic approximation the nonlinear potentials frequently used to model covalent structures can be reduced to this general form. The examples of graphene and diamond lattices are used to determine how adequately these potentials describe the elastic characteristics of the crystals. It is shown that the presented approach allows obtaining natural linkage between the discrete and continuum description of the crystalline solids.

Another way to simulate the nanostructures is using of finite elements method as one of the most powerful computational approaches in continuum mechanics. This method is also frequently applied for the graphene-like calculations. However numerous studies have proved that the microstructure of the material is becoming of the increased importance at the micro and nanolevel. Thus, a theory that can combine the discrete and continuum approaches is needed. In [1] a structural approach to describe the interaction between carbon atoms is proposed. The interatomic bonds are replaced by linear springs of different stiffness. In [1] and the subsequent literature these springs are named rods, however the bending rigidity in these models is not taken into account. Another structural model for nanostructures where the interatomic bonds are simulated by rods with tensile and bending stiffness was proposed in [5], parameters of

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the rods are determined using the known empirical interaction potentials. Models [1], [4] are presented in Fig. 1.

The approach used in the presented work is similar to that of [5], in particular the flexible rods are used to model the interatomic bonds. However an alternative description for the interatomic bonding is used. Instead of the empirical potentials the quadratic form of the vectors describing the relative positions and orientations of particles-atoms is used. Following [3] the parameters of the interaction (namely the values of longitudinal and transverse stiffness of the interatomic bond) are obtained from the values of the macroscopic elastic properties of the corresponding solids. These models were elaborated using two different versions of the mechanical theory of rods, namely Euler-Bernoulli theory and the theory of Timoshenko. The first aim of this work is to obtain correlations between the stiffness of the atomic bonds with the parameters of the rod model. The second aim is to calculate these parameters on the basis of experimental data obtained for the graphene.

The proposed models can be used in standard applications of the finite element software packages or molecular dynamics packages in order to study the elastic properties of graphene, diamond-like structures and carbon nanotubes.

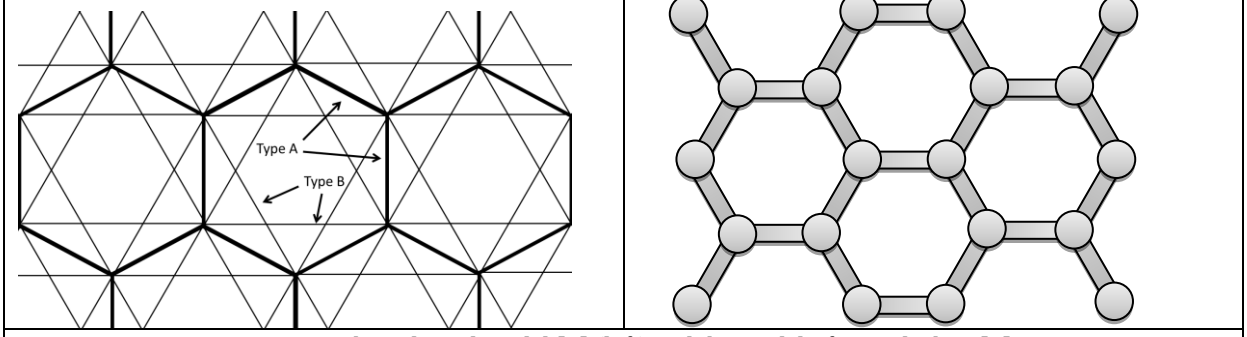

Figure 1. The Odegard model [2] (left) and the model of Li and Chou [5]

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