Nanomechanical properties of polymer composite nanoclusters

Yu.G. Yanovsky*, F.V. Grigoryev[1], E.A. Nikitina,
A.N. Vlasov and Yu.N. Karnet

Institute of Applied Mechanics RAS, Moscow, 119991, Russia
[1] Research Computing Center of Lomonosov Moscow State University, Moscow, 119992, Russia

The paper contains results of quantum mechanical and molecular dynamics simulation of the structure, energy characteristics, and nanomechanical properties of nanoclusters of a "polymer matrix – carbon filler" composite medium. Quantum mechanical simulation is carried out in the framework of the cluster approach, in the approximation of microscopic friction and deformation (tension) for a model polymer – filler boundary layer. Molecular dynamics simulation is performed in NPT- and NVT-ensembles with periodic boundary conditions under normal conditions. Interaction parameters are determined according to the GROMACS force field, the potential energy of rotation about a bond is found from the quantum mechanical simulation results. The simulation findings are used to estimate strength properties of the medium. Based on the data of direct quantum mechanical calculation, we derive approximating dependences for potentials that describe interaction energy in the system "organic polymer matrix – carbon filler particles". The molecular dynamics simulation data are used to calculate the compressibility factor.

Keywords: polymer composites, nanomechanical properties, nanoclusters, quantum mechanical calculations, interaction potentials, molecular dynamics simulation, bulk moduli

1. Quantum mechanical description of nanomechanical properties

1.1. Structure simulation of a basic cluster of the polymer composite

Quantum mechanical calculations are performed by the CLUSTER1 technique designed for parallel computations. This allows simulating, to high accuracy, the spatial structure and interaction energies of molecular systems containing up to 1 000 atoms, that is, several tens of nanometers in size.

A basic composite cluster for the simulation of nanomechanical properties is constructed in the following way. We take two similar particles of irregularly arranged amorphous carbon with pseudoplanar structure (carbon atoms with sp^2-sp^3 electron configurations and differently distributed hole and interstitial dislocations). They are combined with five layers (tree molecules in each layer) of polyethylene oligomers CH_3-$(CH_2)_{14}$-CH_3, which are between two surfaces of the carbon filler particles.

Each carbon particle consists of 176 atoms. Before optimization the parallel planes of two such particles are at a distance of 3 nm. Five layers of the polyethylene matrix are placed between the particles. Each layer is simulated by three polyethylene oligomers CH_3-$(CH_2)_{14}$-CH_3 (50 atoms in each) located at the same level relatively to the carbon particle planes. Thus, the model system contains 1 002 atoms.

Figure 1 represents the quantum mechanically optimized structure of such a complex cluster. It also illustrates calculated geometric parameters (distance in nm between planes and components of the model cluster) necessary for further calculations.

Figure 2 shows parameters (in nm) for the surface area of a carbon particle shielded by a polymer matrix layer, which is calculated using Van der Waals radii of atoms. To normalize the calculated energy of polymer – carbon surface interaction when finding interaction potentials it should be calculated per surface unit of the interphase zone or per monomeric unit of the polymer, which is a -CH_2- group in this case. The monomeric unit size, which is obtained using calculated Van der Waals radii of constituting atoms, is also given in Fig. 2.

1.2. Quantum mechanical calculations of basic cluster deformation

Cluster strain in tension when the two filler particles move relatively to each other perpendicular to the filler

* *Corresponding author*
Prof. Yurii G. Yanovsky, e-mail: iam@ipsun.ras.ru

doi:10.1016/j.physme.2008.11.005

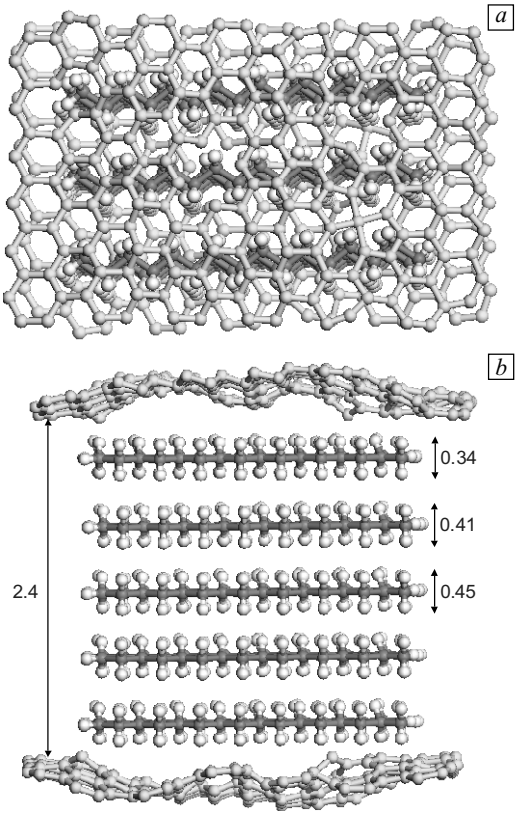

Fig. 1. Quantum mechanically optimized structure of the analyzed nanocluster of the polymer composite: top view (*a*), side view (*b*)

surface plane is calculated in the approximation of the microscopic coordinate of external strain. One (lower) carbon particle is spatially fixed while the other (upper) carbon particle moves away from the first one in the step-by-step

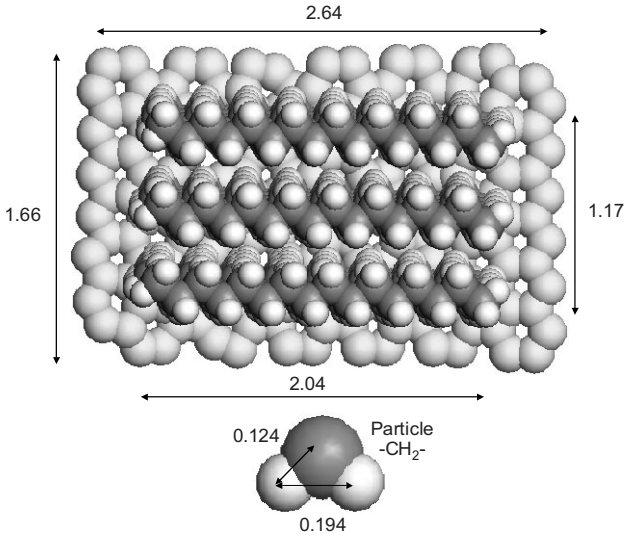

Fig. 2. Basic cluster of the composite in the representation of Van der Waals radii of atoms

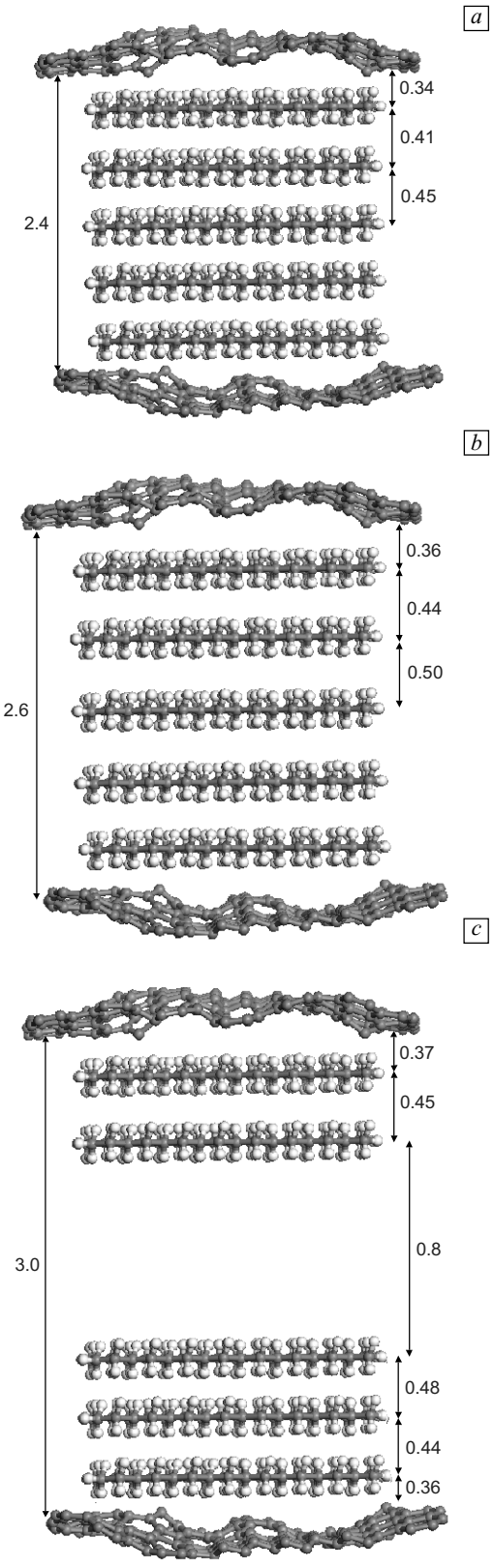

Fig. 3. Sequential simulation steps for deformation of a composite cluster: initial state (non-deformed cluster) (*a*), deformation stages (*b*, *c*)