NOVEL CARBON NANOSTRUCTURES: MOLECULAR AND COVALENT BOUND GRAPHENE-FULLERENE CRYSTALS

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Abstract – Different models based on graphene and fullerens were proposed. Such structures can be obtained from material that was previously synthesized via external influence.

I. INTRODUCTION

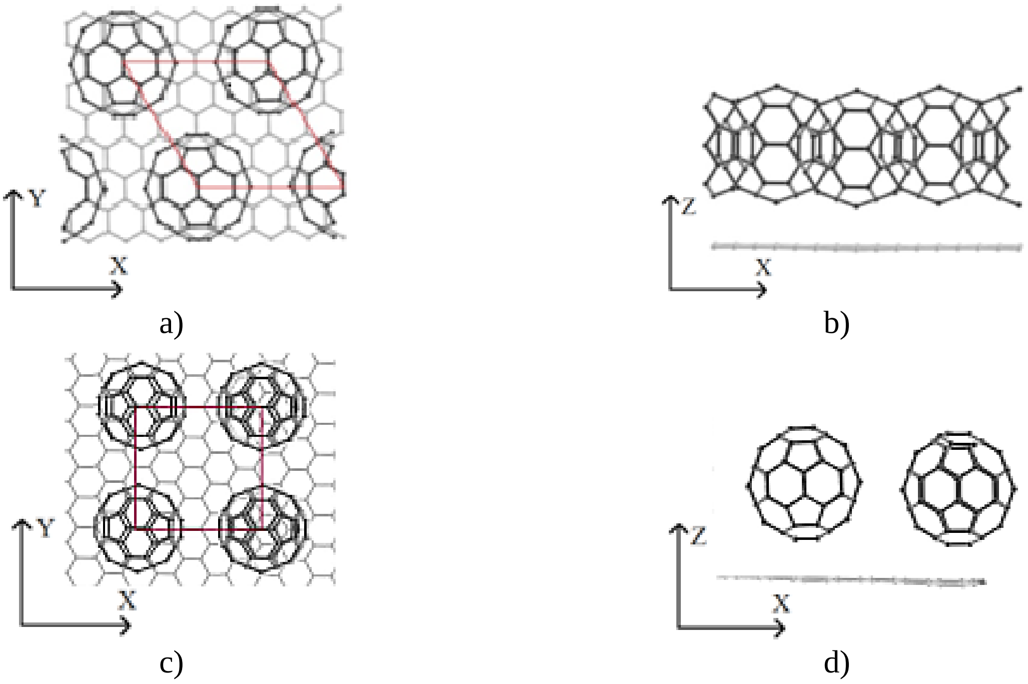
Various graphene-fullerene compounds have been synthesized before [1-4].They are differ from each other by the presence of a covalent bond and the number of graphene layers. In all these works the properties of structure almost were not investigated.

II. SIMULATION METHOD

The mechanical properties of the studied structures were investigated by classical molecular dynamics (MD) method using GULP package [5]. The interaction between carbon atoms was described by Brenner many-body potential [6] which accurately describes the binding energies and elastic properties of wide range of carbon structures [7]. The conjugated gradient method was used for the atomic structure relaxation. For the behaviour investigation of the composite MD simulation method was applied by system at 240, 280 and 500 K during 10 ps with time step of 0.1 fs.

III. COMPOSITE STRUCTURE

As the fullerene monolayer was obtained lying on graphene [4]. We were investigated such model with two different fullerene C_{60} interposition: hexagonal (Fig. 1 a, c) and orthorhombic (Fig. 1 b, d) on graphene surface. The calculation cell is red.



a) b)

c) d)

Figure 1 – Models of fullerene location: a, c – hexagonal, b, d – orthorhombic.

The binding energy was calculated for these structures using next formula:

$$\Delta E_f = (E_s - E_G - NE_f) / N,$$

where E_s- calculation cell energy, E_G – graphene energy, N – the number of fullerenes in calculation cell and E_f – energy of one fullerene.

For hexagonal case binding energy is equalled to -0.88 eV/C_{60}, for orthorhombic - 0.67 eV/C_{60}. It's mean that the composite formation from individual component is energy favourable. The thermal stability was investigated at 240, 280 and 500 K. Observed behavior is similar for fullerite crystal. With decreasing temperature (T <260 K) rotation of fullerene molecules stops. Structure is stable under 500 K.

It is well known that fullerenes is polymerized via [2+2] cycloaddition under temperature, pressure or UV effect [8]. That's why it was interesting to consider the fullerene polymer on graphene substrate and fullerene attached to graphene. The fullerene attaching to graphene is changing binding energy for hexagonal structure up to -11.90 eV/C_{60}, for orthorhombic up to – 11.70 eV/C_{60}.

Sheme of step-by-step connection was investigated for fullerene attached to graphene (Fig.2). On first step there was one pair bond between two fullerene molecules, on second step - two pairs, on third - three pairs, on last - the infinite chain of bonded fullerenes. With number of bond increasing the binding energy is growing. The polymerized state is more energy favorable. Thus we can propose a 3D crystal that is fully polymerized.

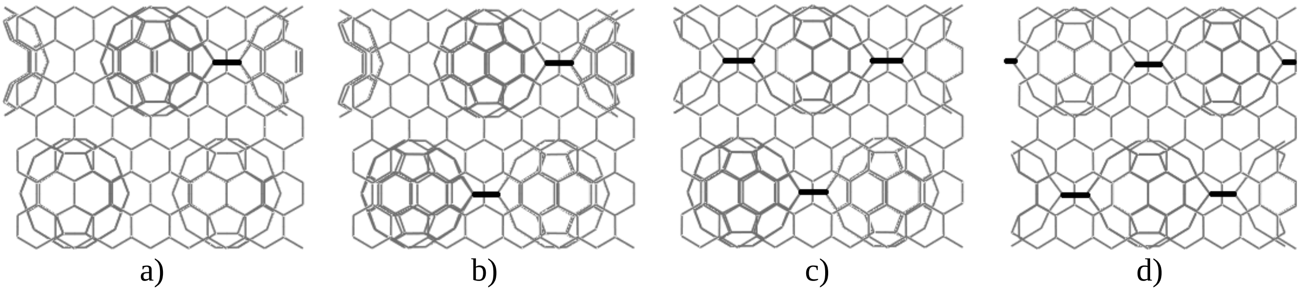


Figure 2 – Scheme of step-by-step connection.

Young's moduli of a 3D structure were calculated using next formula:

$$Y = \frac{F \cdot L}{S \cdot \Delta L},$$

where $F = 2\frac{\partial E}{\partial L}$ – is the force acted on structure.

Here E is the strain energy, L is the structure length and S is the cross-section area of structure. The calculated Young's modulus for XYZ axis are equalled to 0.17, 0.16 и 0.03 TPa. For comparison, Young's module of C_{60} deposited on silicon surface is 0.01 TPa.

IV. CONCLUSION

The new model of polymerized graphene-fullerene structure was considered. Such composite probably can be obtained from compounds [1-4] via exposure that fullerene polymerization promote. The 3D crystal is a stable material with high value of Young's modulus.

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