Computer Simulation of Graphene-Metal Composite Induced by Radiation

A.M.Ilyin*, G.W.Beall**

*National Nanolaboratory, Kazakh National University, Tolebi Str., 96a, Almaty, Kazakhstan, ilyinar@mail.ru

** Center of Nanophase Research, Texas State University San- Marcos, Department of Chemistry and Biochemistry, 601 University Drive, TS USA,gb11@txstate.edu

ABSTRACT

We performed computer simulations and study of graphene with radiation defects, involving vacancies and bridge-like defects, linking with metallic atoms as a model of composite materials. Metal – defect binding energies and structural characteristics have been determined using DFT calculations.

Keywords: graphene, radiation defect, composite, simulation, nanomaterials

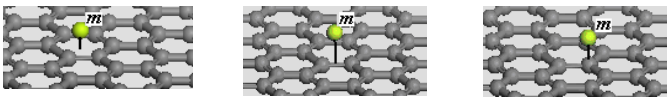
1 INTRODUCTION

Graphene, in spite of its recent availability for experimental investigations [1] is an object of great interest for many researchers because of the very wide fields of its potential applicability: materials science, electronics, sensors, biology, composites etc. In particular, graphene and few layer graphene fragments can be used as elements of reinforcement in production of composites, based on various matrices [2,3]. But well known chemical inertness of graphene results in poor interfacial bonding of the graphene fragments with matrices and limits the level of strength which can be transferred from reinforcing graphene-like elements to the matrix. It is one of the main obstacles in its possible applications for production composite materials. In our recent papers [4-6] we suggested using of radiation bridge-like defects as an effective tool of essential modification of physical-mechanical properties of composites, filled with carbon nanostructures.

Beryllium, aluminum and their alloys are very important materials for designing new composites, especially for fields where combination of light weight with high strength is needed, for example – transportation systems and air-space technologies. Therefore, in this paper we focused on study of possible production composite materials based on Be and Al matrices, with utilizing graphene fragments as reinforcement elements. We propose, that radiation defects might essentially improve binding ability of graphene with atoms of light metals due to production of additional chemical bonds. Unfortunately, direct experimental study of such nanosystems in many cases is practically impossible. These interactions can normally only be measured by indirect measurement of a given property.Therefore in this paper we present some results of computer simulation and calculations by the use of well known DFT technique. Results obtained show that radiation modifying of composite nanomaterials involving graphene and graphene-like structures under special conditions may become a key technology to create very new type of lightweight composites with high mechanical characteristics and useful physical properties.

2 COMPUTER SIMULATION

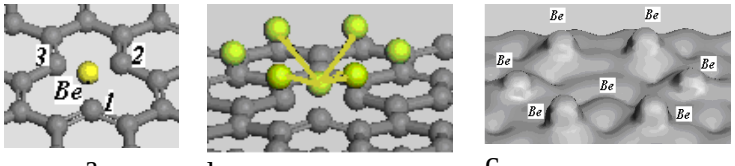
Fig.1 presents some typical configurations of metallic atoms (Be, Al) arranged on graphene surface with binding energy nearly zero.



a b c

Figure 1. Some of calculated symmetrical configurations of metal atoms (Be and Al) on graphene surface with nearly zero binding energies: a) over the center of a hexagon; b) over the center of the C-C bond; c) over a C atom.

2.1 Be -graphene



a b c

Figure 2. Configurations of Be atoms bonded with a vacancy. a) a stable position of the single Be atom in the graphene sheet. The binding energy E_b equals 2.6 eV; b) configuration of an initially flat Be-cluster over vacancy after optimization. The binding energy of the cluster with graphene was obtained as large as 7.2 eV; c) the electron charge distribution in the area of the metal cluster – vacancy with a density of charge 0.2 el / Å^3.

Figure 2 presents possible stable configurations of a single Be atom and of Be-cluster linking with a vacancy. Metal atoms bonded with defect can be considered as roots for joining other metal atoms and creating fast bonds with metal matrix. Here and down in all cases procedures of optimization on energy were performed in order to calculate a possible configuration of a bond of metal atoms with vacancies and bridge-like defects.

Here and down in all cases procedures of optimization on energy were performed in order to calculate a possible configuration of a bond of metal atoms with vacancies and bridge-like defects.

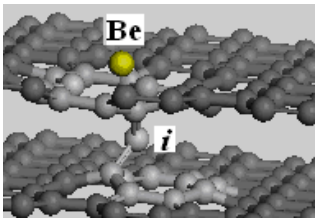


Figure 3. Complex bridge-like radiation defect in bilayer graphene, involving Be atom, placed on the surface. The binding energy of Be atom, is equal to 1.52 eV.

Figure 3 presents a configuration of a more complex defect, involving a bridge-like radiation defect, based on interstitial carbon placed between two graphene sheets and making the nanostructure much more stiffer [5,6]. Calculations show that vacancy zone can also adsorb Be atom with large enough binding energy (E_b = 1.52 eV). This combination is very favorable for creating fast bonding of graphene fragments with matrix.

2.2 *Al* –graphene

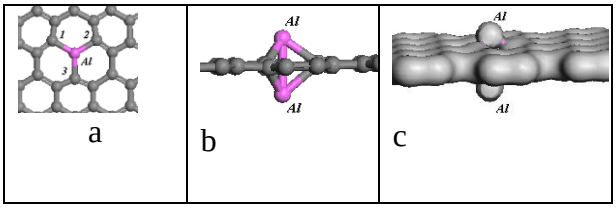


Figure 4.a) *Al* atom – vacancy; b) *Al* - dumbbell bonding with vacancy; c) electron charge distribution with density of charge equals 0.5 el / Å^3.

In all cases, presented in Fig.4 in order of taking into account graphene-size effects, the edges of graphene sheet were fixed during optimization procedure. In the configuration with a single Al (Fig.4,a) there was observing noticeable deformation and spreading of the vacancy zone with Al atom sinking in the sheet of graphene, placing at the symmetrical position. Final distances between Al and the nearest C atoms are: *Al* - C1 and *Al*-C2 : 1.70 Å , *Al*- C3 : 1.71 Å.

Fig.4,b presents a dumbbell of two *Al* atoms, linked with vacancy. The binding energy is equal to 2.9 eV per every *Al* atom with a distance between them 2.5 Å. The distribution of the electron charge in the dumbbell – vacancy complex defect for the charge density 0.5 el / Å^3 is presented in the Fig.4,c.

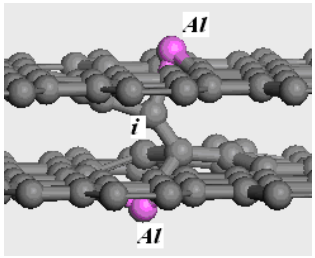


Figure 5.Bridge-like defect with *Al* atoms attached on surfaces. E_b= 1.3 eV.

Figure 5 presents a bridge-like defect, linking two graphene sheets together for stiffening and with two Al atoms attached on both graphene sheets.

We proposed that edges of graphene sheets can also serve as bonding sites for metal atoms creating the additional effect of adhesion with matrix. Two possible stable configurations are presented in Figure 6.

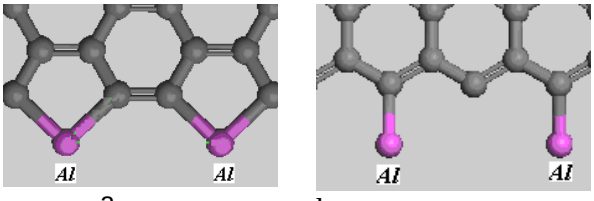


Figure 6.a) possible edge-traps configurations for Al-atoms with the following binding energies: a) 4.2 eV, b) 3.1 eV.

3 CONCLUSION

Some possible types of stable complex defects in graphene fragments, involving vacancies, bridge-like radiation defects and metal atoms (*Be* and *Al*), attached to surfaces, were simulated and calculated using well known DFT technique. Results of calculation show that radiation defects can serve not only as elements of stiffening but also as roots for additional fast chemical bonds with light metal matrices. It proves, that radiation vacancies and bridge-like defects can be very useful tool for technologies of production lightweight composites with high stiffness and strength.

REFERENCES

[1] K.S.Novoselov, A.K.Geim, S.V.Morozov, D.Jiang, Y. Zhang, S.V. Dubonos, I.V.Grigorieva, A.A. Firsov. "Electric field effect in atomically thin carbon films". *Science* 306, 666,2004.

[2] S.Stankovich, D.A.Dikin, G.H.B.Dommett et al. "Graphene-based composite materials". Nature, 442 282-286, 2006.

[3] Ch.Xu, X.Wang and J.Zhu. "Graphene – metal particle nanocomposites". J. Phys.Chem., C, 112 (50) 19841-19845, 2008.

[4] A.M.Ilyin, E.A.Daineko and G.W.Beall. "Computer simulation and study of radiation defects in graphene". Physica E, 42, 67-69, 2009.

[5] A.M.Ilyin and G.W.Beall. "Computer simulation and study of bridge-like radiation defects in the carbon nano-structures in composite materials". NanoTech Conference 2010, June, 21-25, Annaheim, California, USA-2010, Proceedings, P.312-315, 2010.

[6] A.M.Ilyin, G.W.Beall and I.A.Tsyganov. "Simulation and Study of Bridge-Like Radiation Defects in the Carbon Nano-Structures". Journal of Computational and Theoretical Nanoscience , V. **7**, N 10, 2004-2007, 2010.