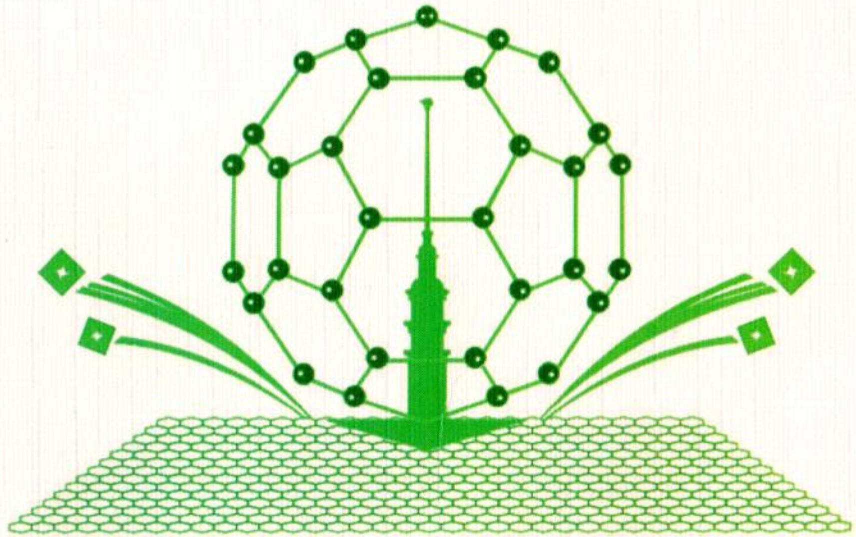
Book of Abstracts

# International Conference Advanced Carbon Nanostructures



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## Electrical properties and structure of amorphous diamond-like carbon nano-sized films embedded with silver and titanium

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Embedding of metal with different chemical nature into amorphous diamond-like carbon (a-C:H) films leads to the appearance of their new physical properties and expands the possibilities of the films practical use [1,2].

It was observed clear pronounced optical plasmon resonance in the visible region in optical absorption spectrum in a-C:H<Ag+Ti> films, as well as in the a-C:H<Ag> films [3], and it was found that the a-C:H<Ag+Ti> films are more thermally stable. At the same time, electrical properties and the structure of the films have not been studied.

Results of electrical properties and structure study of amorphous diamond-like carbon films embedded with silver and titanium (a-C:H<Ag+Ti> films) are presented in this work. The films were prepared by ion-plasma DC magnetron sputtering of the combined target in Ar+$CH_4$ gas mixture. The a-C:H<Ag+Ti> films with thickness from 80 to 100 nm were deposited on quartz and silicon (100) substrates at 50°C. The maximum of Ag and Ti metals concentration in the films reached 4,2 and 20 at. %, respectively, and was changed by alteration of metals and graphite area ratio on the target.

It was found the significant increase in the a-C:H<Ag+Ti> films conductivity ( ~ 10 orders of magnitude) with Ag concentration rise at fixed Ti concentration. Note that percolation character of the concentration dependence of conductivity in the films is less pronounced in comparison with the a-C:H<Ag> films. Temperature dependences of the a-C:H <Ag+Ti> films conductivity, as well as that of the a-C:H<Ag> films, is typical of semiconductors.

Study of the a-C:H<Ag+Ti> films structure by the TEM showed that their matrix contains isolated nanoparticles of silver (~ 60 nm), and those of silver and titanium oxide with dimensions of 2-3 nm. Changes in the electrical properties of the a-C:H<Ag+Ti> films are apparently due to the $sp^3/sp^2$ ratio change of the hybridized bonds in their matrix.

Thus, embedding of Ag and Ti into the a-C:H films could lead to effective modification of their electrical properties with preserve of plasma absorption resonance.

### References

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3. Yu. Prikhodko, S.L. Mikhailova, Ye.S. Mukhametkarimov, et. al, Proc. of SPIE (2016) **9929,** 9929G-1.

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## Structural and electronic properties of nanostructured graphite

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Ab initio simulation of nanostructured graphite was performed using density functional theory. Hybrid system of graphene-$C_{60}$ was used for calculations. We considered superlattice of 116 atoms within the slab scheme. The nearest to the graphene $C_{60}$ pentagon was centered on carbon atom. This configuration corresponds to the minimum of total energy We have performed self-consistent total energy calculations within DFT and pseudopotential method as implemented in [1].

For the exchange-correlation energy we used the PBE functional within the generalized gradient approximation (GGA). For the plain waves used in the expansion of the pseudo-wavefunctions, the cutoff energy was 200 eV. For calculation of all surfaces, we used the k-points generation scheme by the Monkhorst-Pack method with a two-dimensional 4x4x1 mesh. The achieved total energy convergence was at least $10^{-6}$ Ry. Local atomic structure of graphene-$C_{60}$ hybrid system was studied by means of structural relaxation (Fig.1). The electronic energy spectrum of graphene-$C_{60}$ hybrid system was also studied. The effective charges on the nearest neighbor atoms of the fullerene and graphene have been determined.

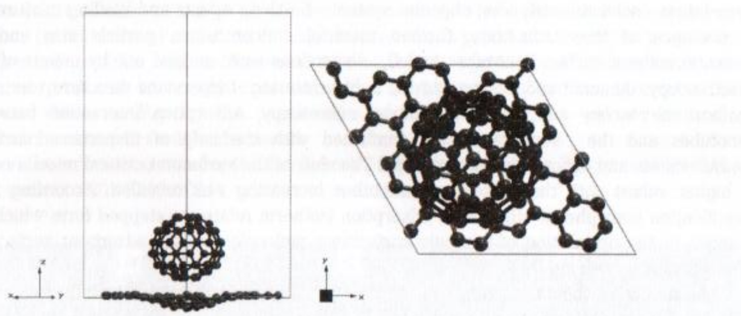

Fig.1. Supercell model of graphene-$C_{60}$ hybrid system after structural relaxation (a - side and b - top views)

### References

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