IMPACT OF NITROGEN ON THE PROPANE-BUTANE/ HELIUM PLASMA COMPOSITION profile ALONG THE JET AXIS [[1]](#footnote-1)\*)

DOI: 10.34854/ICPAF.2020.47.1.147

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Nanodisperse materials synthesized by means of the conversion of different kinds of carbon containing substances from the plasma have a specific composition and phase structures [1].

This work deals with the experimental investigation and the modeling of the plasma jet parameters for the synthesis of graphene doped by nitrogen atoms (N-graphene) and with its characteristics.

The plasma jet was generated using a DC plasmatron with 28-35 kW of power input and with the swirling arc stabilization. Conversion of the mixture made of plasma forming gas (helium with addition of nitrogen) and of the precursor made of a propane and butane mixture was performed under the pressure 350 Torr. Varying the relative flow rates of nitrogen and helium optimal conditions were found for the N-graphene synthesis maximizing its output under the relative mass flow rates of propane and butane 65:35 and the arc current value 350 A.

Modeling of the process was performed in a quasi-one-dimensional approach under the assumption of the local thermodynamic equilibrium. The equilibrium algorithm is based on the minimization of the Gibbs free energy in the space of reaction coordinates by means of the consecutive fitting of reactions and the optimization of basis. All states of substances are accounted – gaseous (including ionized state) and condensed (liquid and solid). At every single step the equation of the law of active masses are solved for the one reaction. Gaseous phase is considered as a mixture of ideal chemically reacting and ionizing gases. For the condensed phase a model of insoluble pure substances is used. Thermodynamic properties of individual substances are imported from the database IVTANTHERMO [2].

The basic set of parameters for the model is the following: helium flow rate – 0.75 g/s, propane-butane flow rate – 0.097 g/s, pressure – 350 Torr. The cooling of plasma along the jet axis is accompanied by the condensation of carbon vapor into molecules C60 and C80. They are absent in the IVTANTHERMO, but may be imported from the publication [3], where they are identified as fullerene and soot.

An addition of nitrogen to the carrier gas (helium) overturns the plasma composition. In place of C60 and C80 there appear cyanopolyynes HC9N and HC11N loaded by the lot of carbon atoms.

Inadequate fitting of results of modeling to the experiment is due rather to the lack of experimentally observed structures in the set of individual substances than to the breach of the local thermodynamic equilibrium, because the pressure is high enough (350 Torr).

The project is supported by Russian Foundation for Basic Research, grant 19-08-00081.

References

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2. Belov G.V. et al. High Temperature, 2000, 38, 191.
3. Esfarjani S.A. PhD thesis, University of Toronto, 2013.
1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/XLVII/Pt/ru/GB-Shavelkina.docx) [↑](#footnote-ref-1)