KINETIC ANALYSIS OF HYDROCARBON CONVERSION IN THE VOLUME OF A PLASMA JET DURING GRAPHENE SYNTHESIS [[1]](#footnote-1)\*)

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One of the common methods for obtaining nanocrystalline powders is gas-phase synthesis. In this case, chemical processes occur near or on a cold surface, which limits the productivity of the method and makes the properties of the synthesis products dependent on the substrate material. To improve the quality of nanostructures and the productivity of the method, it is proposed to use gas-discharge plasma as a medium. The method is based on the decomposition of hydrocarbons in plasma jets generated by a DC plasma torch at a pressure somewhat below atmospheric. To synthesize a specific carbon nanostructure under given conditions, it is necessary to determine the key chemical reactions, the temperature range for their efficient occurrence, the composition of the intermediate conversion products, and the temperature profile.

The purpose of this work was to find the leading reactions for different initial gas compositions; the final composition of the mixture; dependence of gas-phase products on the nature of the carrier gas and the temperature profile along the plasma jet. The composition of the final and intermediate (along the jet) products obtained as a result of the kinetic approach was compared with the results obtained within the framework of the thermodynamic approach. Three compositions were considered: I - CH4/N2, II - C3H8/C4H10/He и III - CH4/Ar at the same pressure *P*=350 Torr. The maximum temperature at the nozzle exit varied in the range of 8000–10000 K, the conversion in the jet took place within ~1 s, and the temperature profiles were different (different jet cooling rates). In experiments [1], under the above conditions for mixture III, low-defect nanostructures with a lateral size of up to 2000 nm are formed at the outlet of the reactor, which is much larger than their geometry during synthesis for other mixtures.

As a result of kinetic calculations, differences in conversion for the three mixtures were revealed. For mixture II, the electron concentration at the nozzle exit was almost an order of magnitude lower than for mixtures I and III. This is due to the fact that the ionization potential of helium is much higher than for nitrogen and argon. Ion-molecular and electron-ion reactions play a role during the first few milliseconds. The main chemical reactions that affect the appearance of nuclei from C2 molecules as a result of the formation of supersaturated vapor and the precipitation of a solid phase occur in the range *T*=4000–2500 K with the participation of the C2H radical [2]. The end products in the gas phase are H2 and C2H2. For mixture III, the jet had a sharp cooling rate, and the mixture already had *T*~4000 K by *t*=35 ms. The temperature range of 4000–2500 K lasted ~200 ms. For mixtures I and II, the duration of this range was approximately the same, however, the moment from *T* ~ 4000 K came to 380 ms. As a result, for mixture III, there was much more time for the growth of solid nanoparticles, since the first nuclei formed much earlier. C2H, C2, and the carbon solid phase (in total, including graphene) behave similarly in the thermodynamic calculation, where their growth began at *T*~3200 K and stopped at *T*~2500 K, i.e. when C2H disappears from the volume, and, accordingly, C2, however, at *T* = 4000-2500 K, there is not enough time to achieve thermodynamic equilibrium.

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References

1. Shavelkina M. et al. J. Materials, 2020, v.13, p.1728.
2. Shavelkina M.B., Filimonova E.A., Amirov R.Kh. PSST, 2020, v.29, 025024.
1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/L/Pt/ru/GC-Filimonova.docx) [↑](#footnote-ref-1)