NEW METHODS FOR SYNTHESIS AND MODIFICATION OF NANOCARBONS

^a <u>Krasnikov D.V.</u>, ^{a,b} Khabushev E.M., ^{a,b} Novikov I.V., ^aGrebenko A.K., ^{a,b}Bogdanova A.R., ^a Alekseeva A.A., ^a Ramirez J.A.B., ^a Raginov N.I., ^a Iakovlev V.Ya., ^{a,b} Nasibulin A.G.

^a Skolkovo Institute of Science and Technology, Moscow, Russia ^b Aalto University School of Chemical Engineering, Espoo, Finland

Being one of the few elements known since prehistoric times, carbon has been continuously modified throughout history: through understanding the phenomenon of allotropy (graphite/diamond) and the theory of the structure of organic species (a vivid example is the detective story of determining the structure for benzene) to self–organizing dissipative systems (fullerenes) and two-dimensional materials (graphene). A wide range of applications of carbon nanomaterials includes antistatic and functional coatings, reinforced materials, as well as smart surfaces and sensors providing a high commercial interest. At the same time, a constantly updated list of new promising solutions in the field of medicine (drug delivery and biocompatible electrodes), telecommunications (single-photon emitters and terahertz optics), robotics (sensitive elements and elastic electronics of artificial skin) explains the special attention from the scientific and technological community.

The present work is devoted to the creation of carbon nanomaterials with tailored characteristics as well as corresponding devices. An important aspect of the work is a development of a new type of continuous reactors for chemical vapor deposition on the surface of an aerosol catalyst. In contrast to classical methods relating to metalorganic volatile compounds, we implement a tandem approach using an aerosol spark discharge generator of catalytic particles. We show that the proposed method not only provides nanotubes with characteristics comparable to classical approaches, but also facilitates the scaling of the reactor by separating the zones of generation of catalytic particles and catalytic process. Moreover, the optimal activation conditions and residence time of the catalyst were determined, which allowed an order of magnitude increase in the productivity of the process and a gain in the quality of nanotube-based transparent electrodes.

A deep understanding of the processes on the surface of the catalyst during the Boudouard reaction yielded a breakthrough process for obtaining graphene, a material associated with the development of new-generation electronics. However, the unique properties of graphene are incompatible with defects in its structure including grain boundaries. Recently, we proposed a simple technology for producing graphene using carbon monoxide as a source under atmospheric or elevated pressure. At the same time, the size of graphene crystals was limited only by the laboratory scale reactor (several cm), and the material was of a single layer only.

At the same time, to "solve" the complex and multiparametric process of synthesis of single-walled carbon nanotubes (one of the central tasks of nanotechnology over the past 30 years) a new approach was proposed. In the works of the applicant, the possibility of integrating machine learning methods for predicting synthesis results (as well as its advanced optimization) was shown for the first time. The developed technology is the key for the industrial processes with autonomous optimization and selection of parameters, which in the future will reduce the costs of the corresponding devices. It is important to note that the accumulated results allowed not only to develop a fundamental understanding of the processes occurring on the surface of the catalyst and carbon nanomaterials but to implement a number of elastic electronics devices with improved characteristics (conductive electrodes, regenerated protective membranes, mechanical sensors, THz optics components). Moreover, this resulted in a multiplicative effect for related fields (photonics and telecommunications (in particular fiber lasers and emitters), sensors (gas sensors), and electronics (elastic LEDs).

This work was supported by the Russian Science Foundation grant No. 20-73-10256 and the Council on grants of Russian Federation (grant number HIII-1330.2022.1.3).