

Рисунок 5 – Геометрическая структура полученных соединений трития в системе.

#### ЛИТЕРАТУРА

1. Soler, J.M. The SIESTA method for ab initio order-N materials simulation / Soler J.M., Artacho E., Gale J. D., Garcia A., Junquera J., Ordejón P., Sanchez-Portal D. // Journal of Physics: Condensed Matter – 2002. – 14, 2745.
2. Cantor, S. Viscosity and Density in Molten BeF<sub>2</sub>–LiF Solutions / Cantor S., Ward W.T., Moynihan C.T. // The Journal of Chemical Physics – 1969. – 50, 2874.

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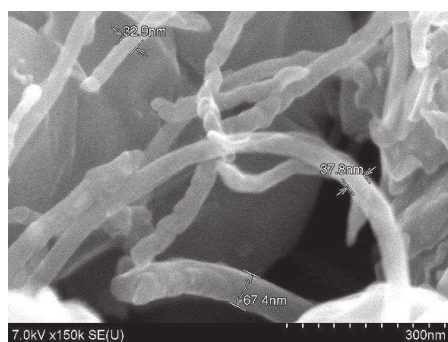
### CARBON NANOTUBES' PERFORMANCE OF SUPERCAPACITOR

The carbon nanotubes (CNT) are widely used for electronics, hydrogen sorption, sensors and catalysts. But the supercapacitors must pursue high bulk energy density, and the electrode materials must be compacted. CNT get the characteristics of excellent conductivity and thermal conductivity, high chemical stability and large specific surface area, which is a very important research direction in the field of electrode materials for supercapacitors. It is expected to provide reference for the development of high-performance carbon supercapacitors.

However, CNT and graphene are easily agglomerated materials due to their large specific surface area, and the loss of easily accessible specific surface area leads to the decline of capacitance performance [1]. Furthermore, the practical use of CNT is constrained by an unavailability of controllable methods of CNT purification, activation and modification. The problem consists in an organization of technologically and technically possible methods of CNT activation and estimation of its efficiency [2].

The purpose of this work is a study of electrochemical, capacitor properties and morphological structure of CNT after their chemical treatment in concentrated nitric acid and hydrogen peroxide.

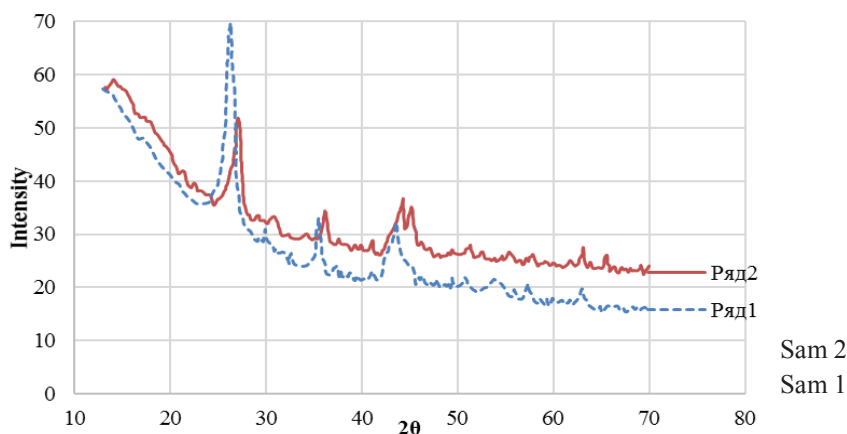
The CNT were obtained in the generator of low-temperature plasma in LLC "Advanced research and technology" (Minsk). The initial materials were the methane-air mixtures, which were injected in plasma stream. The flow consumption of mixture was achieved 1.5 m<sup>3</sup>/h in methane and 4 m<sup>3</sup>/h in air. The power of generator was 28 kW. Thus, the initiated reactions of partial oxidation and pyrolysis of hydrocarbons led to formation of the structured carbon forms on hot reactor walls. The deposit (the sample No.1) of the structured carbon was periodically gathered for the further use. The obtained deposit was a black carbon powder 0.2 g/cm<sup>3</sup> in bulk density. According to the scanning electronic microscopy it was consisted of carbon nanotubes 32-67 nm in diameter, nanofibrils and amorphous carbon (Fig.1).



**Fig 1. SEM image of CNT (the sample No.1)**

For the treatment of carbon nanotubes, the sample No.2 was accurately weighed 0.2 g of CNT and dissolved in 50 ml of 20% sulfuric acid solution, then 63% concentrated nitric acid was slowly added and all mixture was heated on the electric furnace to 90 °C and held in 2 hours.

The phase structure of the material was characterized by X-ray diffraction (XRD)



**Fig. 2 XRD spectra of the carbon nanotubes before and after treatment**

Graphene shows great similarity in XRD with CNT and joints, respectively, for the main peaks at  $\approx 24$  and  $43^\circ$  [3, 4, 5]. Generally, for carbon nanotubes, the first peak at the right refers to crystalline or amorphous nature; thus, the width increases with reducing intensity or length, which refers to exist in amorphous crystal form [6].

The energy dispersive X-ray analysis of CNT were carry out by energy dispersive X-ray Microanalysis together with scanning electron microscopy. When using energy dispersive X-ray analysis [8] of large-scale CNT should be avoided since it may cause error in identification due to overlap of peaks for CNT with many elements such as Fe K $\alpha$ , Si K $\alpha$ , Ti K $\alpha$ , Cr K $\alpha$ , Ni K $\alpha$ , Cu K $\alpha$ , see Tabl. 1.

**Tab. 1 - The energy dispersive X-ray analysis of the CNT before and after treatment**

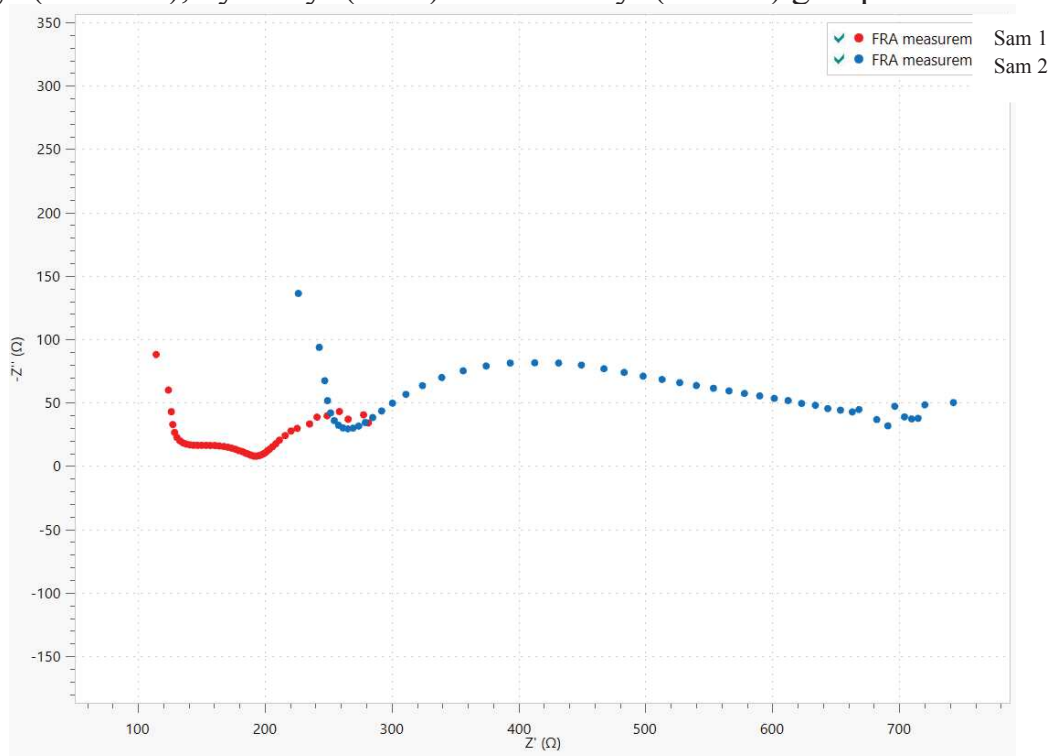
Element	Sample No1 mass%	Sample No 2 mass%
C K	93,58	93,46
O K	2,91	4,79
Si K	0,32	0,32
Ti K	0,23	-
Cr K	0,78	0,39
Fe K	1,41	0,56
Ni K	0,25	-
Cu K	0,53	0,48

The analysis showed two peaks corresponding to C K $\alpha$ , O K $\alpha$ , respectively, related to the presence of C, and O elements in the sample No.1 and the sample No.2. The quantitative analysis for carbon nanotubes before and after treatment confirms that the percentage weight of C, which corresponds to CNTs, was lost 0.12%. It cannot be used to determine amorphous carbon content. [5]. The O refers to the groups of oxide which are produced by a purification process by using nitric acid.

Expression peaks were observed at  $2923\text{ cm}^{-1}$  and  $2850\text{ cm}^{-1}$  in the absorption infrared spectra of pristine and modified carbon nanotubes reflecting fluctuations of C-C and C-OH bonds. The peak at  $1716\text{ cm}^{-1}$  corresponds to the C=O bond, which is characteristic of ketonic, carboxyl and lacton groups. They can catalyze electrochemical hydrogen adsorption and reduction processes. The expression peaks at  $1578\text{ cm}^{-1}$  and  $890\text{ cm}^{-1}$  are caused by deformation of the aromatic structure. The largest peak at  $1200\text{ cm}^{-1}$  most likely corresponds to phenolic oxygen. Compared with sample 1, sample 2 is characterized by a peak at  $1630\text{ cm}^{-1}$ , indicating the presence of a large number of C=C bonds. The smooth peaks corresponding to aro-

matic structures and  $sp^2$  C–H bonds most likely reflect the removal of amorphous carbon structures during the activation modification of CNTs.

CNTs were found to have lower impedance, which was attributed to higher material retention during filtration. Figure 9 shows that the impedance magnitude of CNT No. 1 is much lower than that of No. 2. This is determined by the functionalization of nanotube surface groups such as carboxyl ( $-\text{COOH}$ ), hydroxyl ( $-\text{OH}$ ) and carbonyl ( $=\text{C}=\text{O}:$ ) groups.



**Fig 3. Impedance diagrams of CNTs in 20%  $\text{H}_2\text{SO}_4$**

The study showed that the samples produced by drying the carbon nanotubes all showed an RL equivalent network in series with another resistor as part of the RC segment. This interesting high-frequency sensing behavior is attributed to the wrapping of nanotubes around the pores of the paper substrate [9]

The electrochemical performance of the three-electrode system was tested on an electrochemical workstation, and the prepared electrode was used as a research electrode for cyclic voltammetry with a scan rate of 5-100 mV/s. The specific capacitance varies by several orders of magnitude from  $\sim 0.01$  F/g to  $\sim 50$  F/g at scan rates of 5-100 mV/s, and it is not significantly affected by electrode quality, but varies with material composition and electrolyte. Although the thickness of the electrodes is not commonly reported in the literature, this suggests that the specific capacitance does not depend critically on the electrode thickness.

## REFERENCE

1. Advantages and challenges of using carbon nano-materials for 4V supercapacitors [C] / Qian Weizhong [et al.] // Proceedings of the 2015 annual meeting of the Chinese Chemical Society. – 2015. – P. 18-58.
2. Sadek E.M. Carbon nanotubes and other carbon nanomaterials: Prospects for functionalization / E.M. Sadek, S.M. Ahmed // Proceedings of the New Jersey Institute of Technology – 2023 – P. 107-147.
3. Carbon nanotubes characterization by X-ray powder diffraction – A review / Rasel D. [et al.] // Current Nanoscience. – 2015. – N. 11.– P. 23-35.
4. X-ray diffraction patterns of graphite and turbostratic carbon / Li Z.Q. [et al.] // Carbon. – 2007. – V. 45, N. 8. – P. 1686-1695.
5. Johra F T. Facile and safe graphene preparation on solution based platform / Johra F.T., Lee J.-W., Jung W.-G. // Journal of Industrial and Engineering Chemistry.– 2014. – N. 20. – P. 2883-2887.
6. Designed synthesis of tunable amorphous carbon nanotubes (a-CNTs) by a novel route and their oxidation resistance properties / Longlong X. [et al.] // Bulletin of Materials Science. – 2014. – V. 37, N. 6. – P. 1397-1402.
7. Yoon T.H. Applications of soft X-ray spectromicroscopy in material and environmental sciences / Yoon T.H. // J. Appl. Spectr. Rev. – 2009. – V.44, N.2. – P. 91-122.
8. Scanning Electron Microscopy and X-ray Microanalysis / Goldstein J. [et al.]. – Berlin: Springer, 2003. –356 p.
9. Muhlbauer, R.L. The effect of substrate pore size on the network interconnectivity and electrical properties of dropcasted multiwalled carbon nanotube thin films. / Muhlbauer, R.L.; Joshi, S.; Gerhardt, R. // J. Mater. Res. – 2013. – N. 28. – P. 1617–1624.