



ХІІІ МЕЖДУНАРОДНЫЙ СИМПОЗИУМ
ПОЛУЧЕНИЮ ВЗРЫВОМ НОВЫХ МАТЕРИАЛОВ:
НАУКА, ТЕХНОЛОГИИ, БИЗНЕС И ИННОВАЦИИ
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THERMAL ANALYSIS OF DETONATION NANODIAMONDS

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ОБЪЕДИНЕННЫЙ

ИВТРАН



nanodiamonds

In this work investigated nanodiamond powder has been produced from mixture of TNT and RDX (50/50) by the explosion method [1]. Diamond blend (the condensed product of detonation synthesis) has been subjected to the acid treatment and chemical cleaning. The metal impurities have been removed from the blend by the method of the acidizing. The carbon impurities containing the carbon-like phase have been removed by the thermal oxidation at 350 °C for 4 hours.

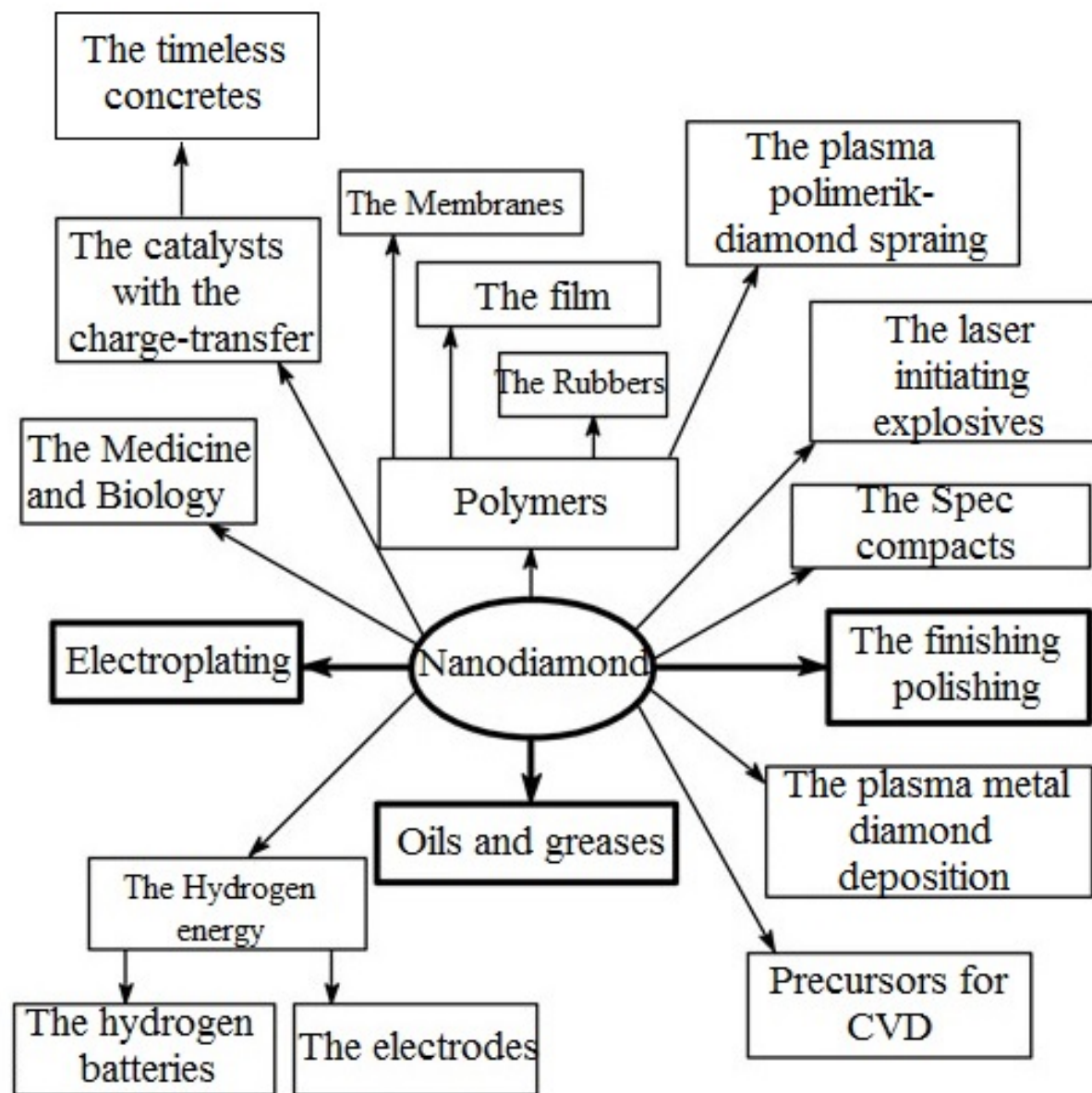
The chemical cleaning of the diamond blend has been performed by the barothermal method in the reactor with the nitric acid at the temperature of 240 °C and the pressure of several tens of atmospheres. The purified product has been washed and dried in the thermostat at the temperature of 100 °C.

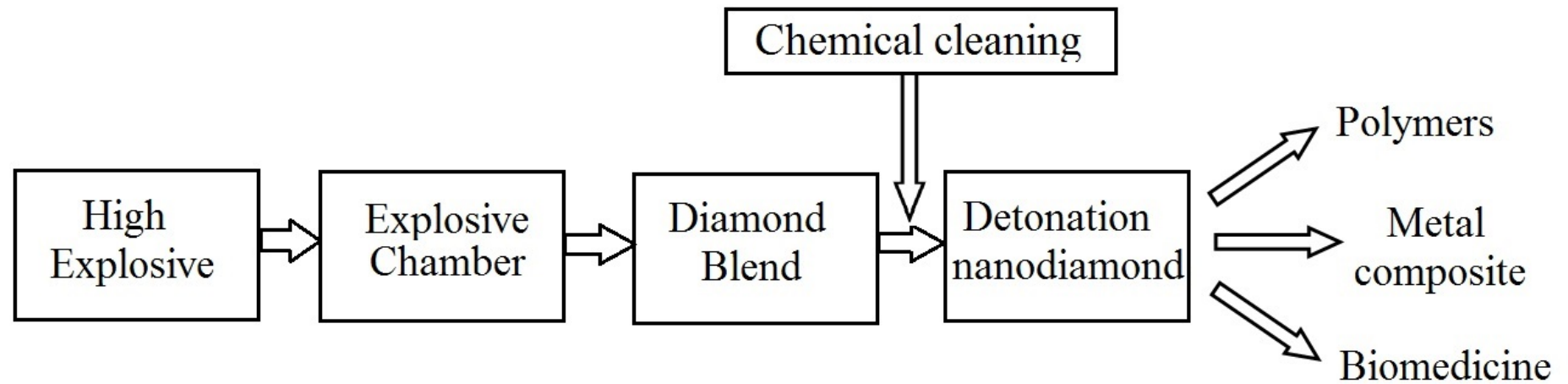
The elemental composition of the DND after the purification is presented in table. The purity of carbon is over 98%, as it was determined by the X-ray diffraction (Table).

The study of our detonation nanodiamonds by the transmission electron microscopy showed that the particles have diameter from 4 nm to 6.6 nm].

1. Шевченко Н.В., Горбачев В.А. Перспективы промышленного получения детонационного наноуглерода. Международная НП конференция “Промышленная утилизация вооружения, специальной техники и боеприпасов”. г. Москва. “ИТЕРПОЛИТЕХ-2012”. С. 335 - 343

POSSIBLE APPLICATIONS OF DETONATION NANODIAMONDS





**WHAT THE BEST APPLICATION OF
DETONATION NANODIAMOND?**

Why the application of the detonation nanodiamonds have not been found yet?

- The laborious technology of the purification of detonation nanodiamond;
- A small percent of its content in the starting material ("diamond blend");
- The high polydispersity;
- The **main obstacle** is the non-reproducibility of the obtained product in the batches: different particle size, different chemical and functional compositions, and etc.

Application of detonation nanodiamond:

- composite

materials -[3] **Behler K D** et al. Nanodiamond-polymer composite fibers and coatings // ACS Nano. 2009. V. 3. Pp. 363–369.

-[4] **Cheng J L** et al. Facile approach to functionalize nanodiamond particles with V-shaped polymer brushes// Chem. Mater. 2008. V. 20. Pp. 4224–4230

-[5] **Mochalin V N** et al. Covalent incorporation of aminated nanodiamond into an epoxy polymer network // ACS Nano. 2011. № 5. Pp. 7494–7502.

- biomedicine-[6] **Rosenholm J.M., Vlasov I.I., Burikov S.A., Dolenko T.A., and Shenderova O.A.** Nanodiamond-Based Composite Structures for Biomedical Imaging and Drug Delivery // J. Nanosci. Nanotechnol. 2015. V. 15. Pp. 959 – 971.

- the metal

matrix-[7] **Popov V.A.** Metal Matrix Composites with Non-Agglomerated Nanodiamond Reinforcing Particles composites // Nova Science Publishers. 2013. Pp. 369-402

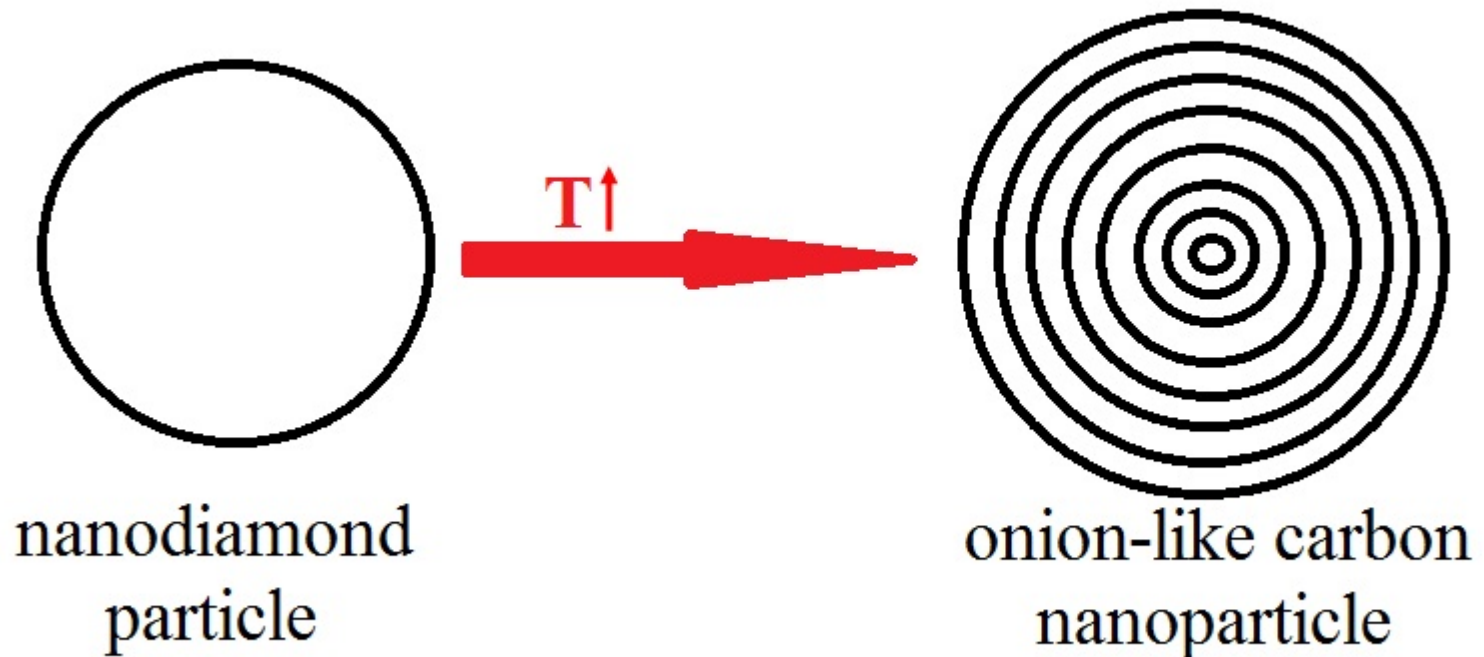
THE MOTIVATION

Temperature of the beginning of graphitization T, °C	References
670	[8] Xu NS, Chen J, Deng SZ. // Diamond and Related Materials. 2002. 11. Pp. 249–56.
>927	[9] Dolmatov V. Yu // Uspehi himii. 2001. V. 70. № 7. Pp. 687 - 708.
>800	[10] Chen, S. Z. Deng, Jun Chen, Z. X. Yu, and N. S. Xua // Applied Physics Letters. 1999. V. 74. № 24. Pp. 3651 - 3653.
927	[11] Aleksenskiy A.E., Baydakova M.V., Vul A.Ya., Davyidov V.Yu., Pevtsova Yu.A. // Fizika tverdogo tela. 1997. V. 39. № 6. Pp. 1125 - 1134.

Today, the thermophysical data of the detonation nanodiamonds are enough contradictory. For composites and alloys obtaining it is necessary more special work to systematization and correction this data.

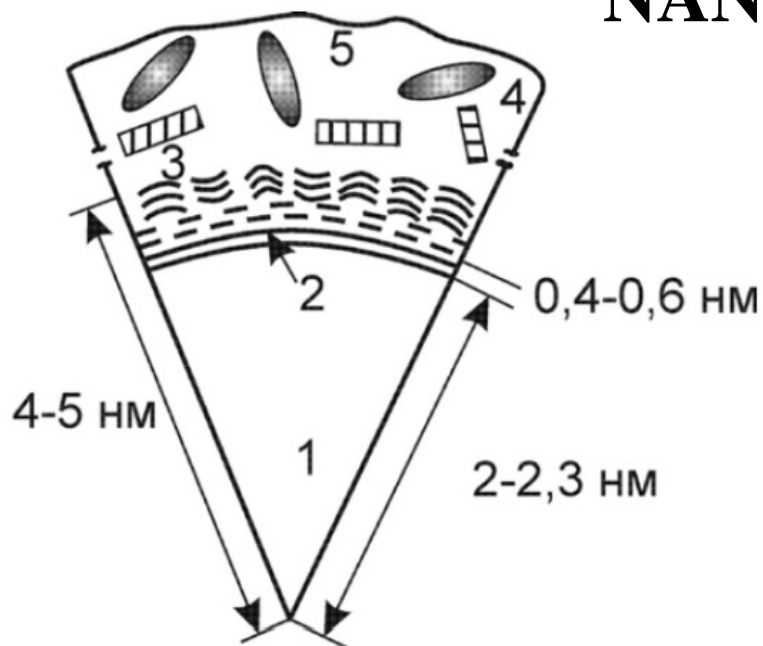
[1] Efremov V.P., Zakatilova E.I., Maklashova I.V., Shevchenko N.V. Svojstva detonacionnyh nanoalmazov pri povyshennyh temperaturah // Konstrukcii iz kompozicionnyh materialov. 2016. Will be published.

THE MODEL OF THE DESTRUCTION NANODIAMOND PARTICLE



[12] Popov V.A. Metal Matrix Composites with Non-Agglomerated Nanodiamond Reinforcing Particles composites // Nova Science Publishers. 2013. Pp. 369-402

STRUCTURE AND SIZE OF THE DETONATION NANODIAMOND



Model of the structure a particle of detonation nanodiamond: **1)** Diamond core **2)** Carbon layer Onion-like, **3)** Graphite nanoplatelets, **4)** The graphite particles, **5)** Inclusion of the metal oxides.

Dependence of the diameter (D) nanodiamond particle as function of atoms (N_{at}).

D , nm	2,2	2,4	2,6	2,8	3,4	3,8	4	4,2	4,6	5	6	6,6
N_{at} , $\cdot 10^3$	1	1,3	1,6	2,0	3,7	5,2	6,01	6,95	9,14	11,74	20,3	27,00

THE PHASE DIAGRAM OF NANOCARBON

The formation enthalpy of the nanoparticles:

$$H(T, p) = H^*(T, p) + \Delta(\Delta_f H_{298}^0)$$

$\Delta(\Delta_f H_{298}^0)$ - the excess formation enthalpy of the detonation nanodiamonds particles[13]

The entropy of the nanoparticles:

$$S(T, p) = S^*(T, p) + \Delta S$$

ΔS - the excess entropy of the detonation nanodiamonds particle[13]

The equation of the line of phase equilibrium:

$$\mu_1(p, T, \Delta(\Delta_f H_{298}^0)_1) = \mu_2(p, T, \Delta(\Delta_f H_{298}^0)_2)$$

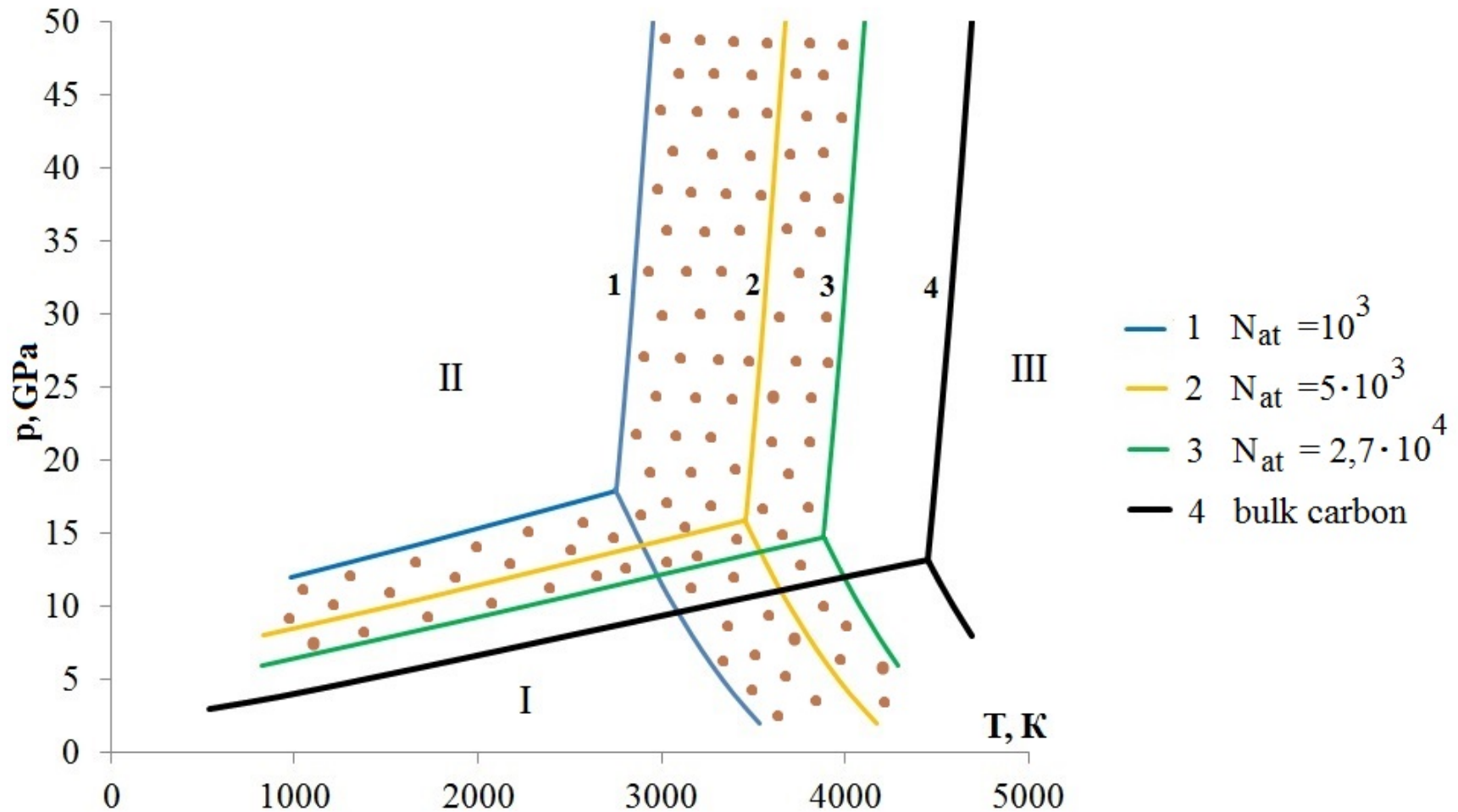
$$G_1(p, T) - G_2(p, T) - (\Delta H_{12} + \Delta S_{12} \cdot T) = 0$$

$$\Delta H_{12} = \Delta(\Delta_f H_{298}^0)_1 - \Delta(\Delta_f H_{298}^0)_2$$

$$\Delta S_{12} = \Delta S_1 - \Delta S_2$$

[13] Gubin S.A. , Maklashova I.V. , Dzhelilova E.I. On the free of size, shape, and internal structure on phase equilibrium in graphite and diamond nanocrystallites // Nanotechnologies in Russia, 2015, Vol. 10, Nos. 1–2, pp. 18–24

THE PHASE DIAGRAM OF CARBON

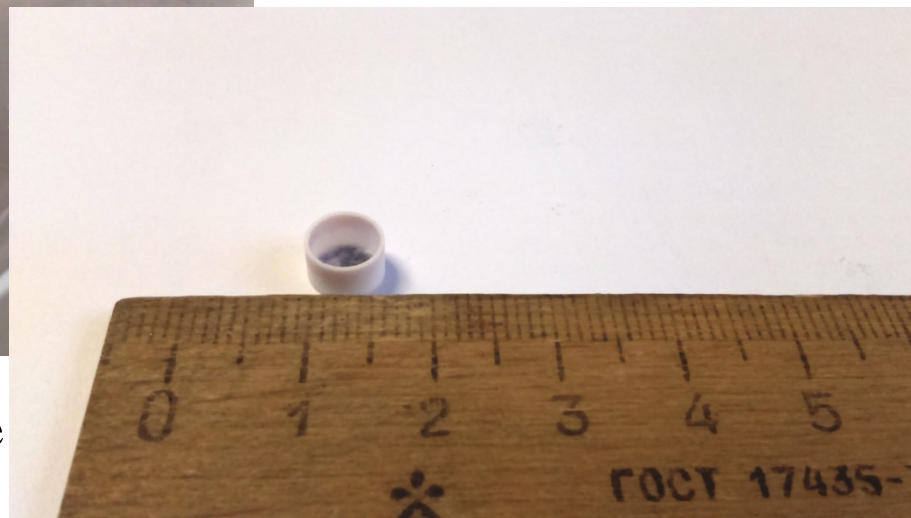


The phase diagrams for nanocarbon, depending on the size of the nanoparticles: $I - N_{\text{at}}=10^3$; $2 - N_{\text{at}}=5 \cdot 10^3$; $3 - N_{\text{at}}=2,7 \cdot 10^4$; $4 -$ bulk carbon. Areas of thermodynamic stability: I – graphite, II – diamond, III – liquid carbon. (N_{at} - the number of atoms in the nanoparticle).

METHOD OF THE STUDY

- The *synchronous thermal analysis* (STA) which includes the *thermogravitation measurements* (TG) and the *differential scanning calorimetry* (DSC) on the device Netzsch STA 409 PC
- The X-ray diffraction
- The scanning electron microscope

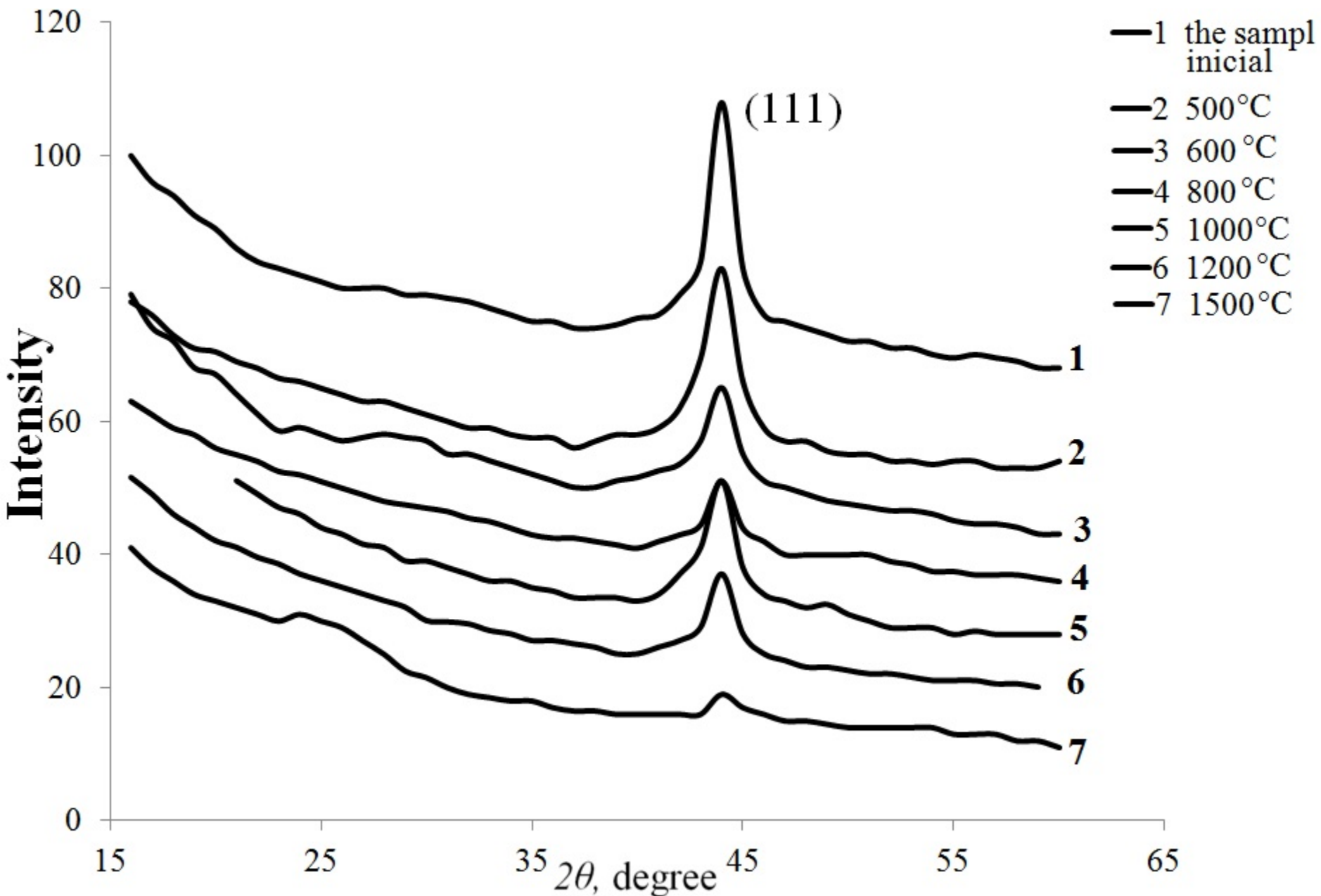
METHODS OF THE STUDY



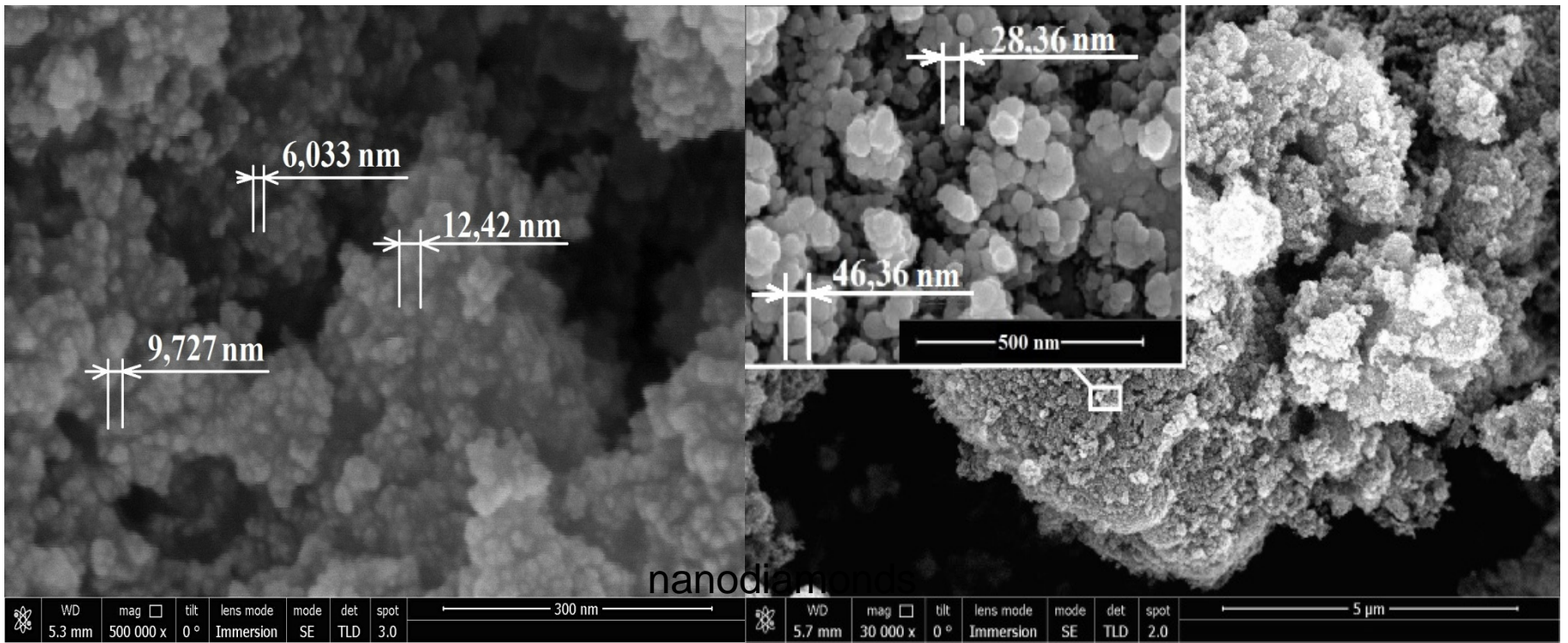
The crucible with the sample of detonation nanodiamond

Element structure of the cleared detonation nanodiamond.

C	Fe	Cr	Ti	Ba	Cl	S	Si	Al	Cu	Ca	K	Mg	Na
98.6	0.30	0.22	0.20	0.04	0.02	0.02	0.02	0.03	0.32	0.02	0.03	0.04	0.13



The diffractograms of the sample after the first heating with the rate 10 K/min



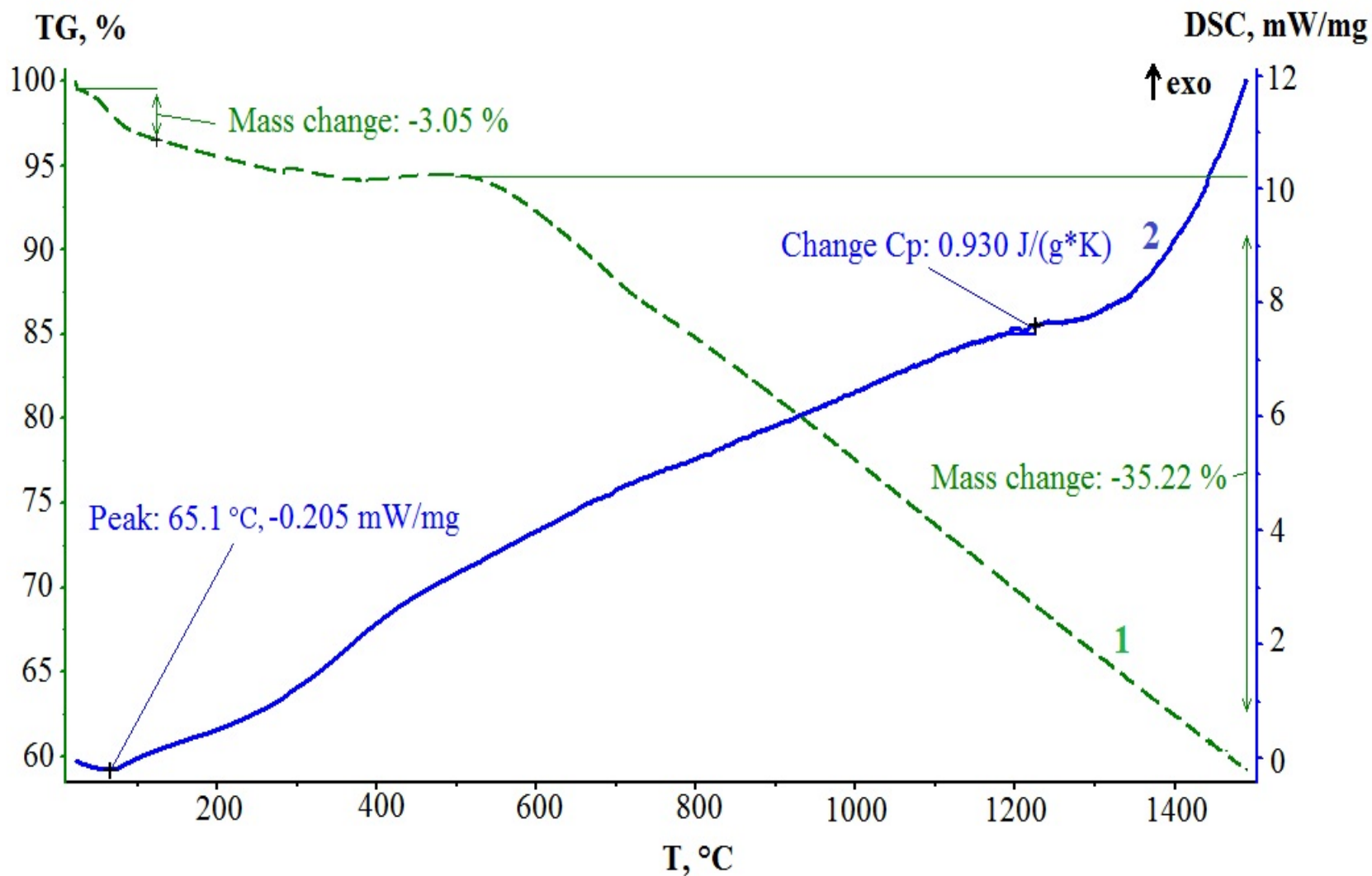
a)

b)

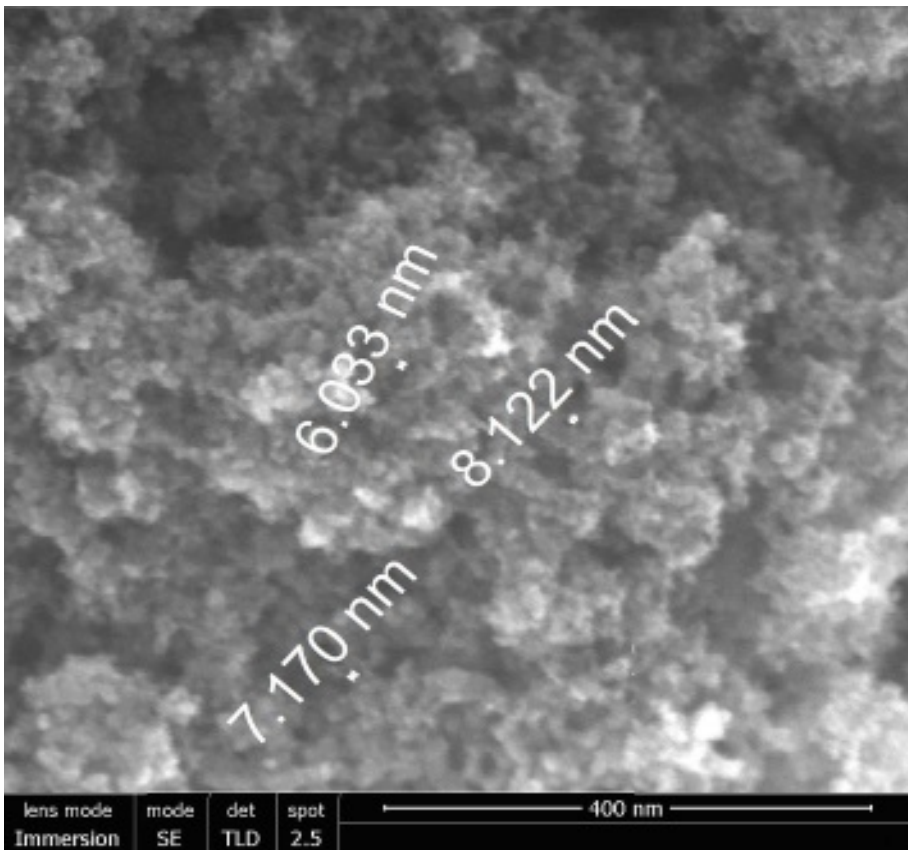
Microstructure of the sample detonation nanodiamond before (a) and after (b) of the heat treatment (temperature 1500 °C with the rate 10 K/min).

We are suggesting method of secondary heating

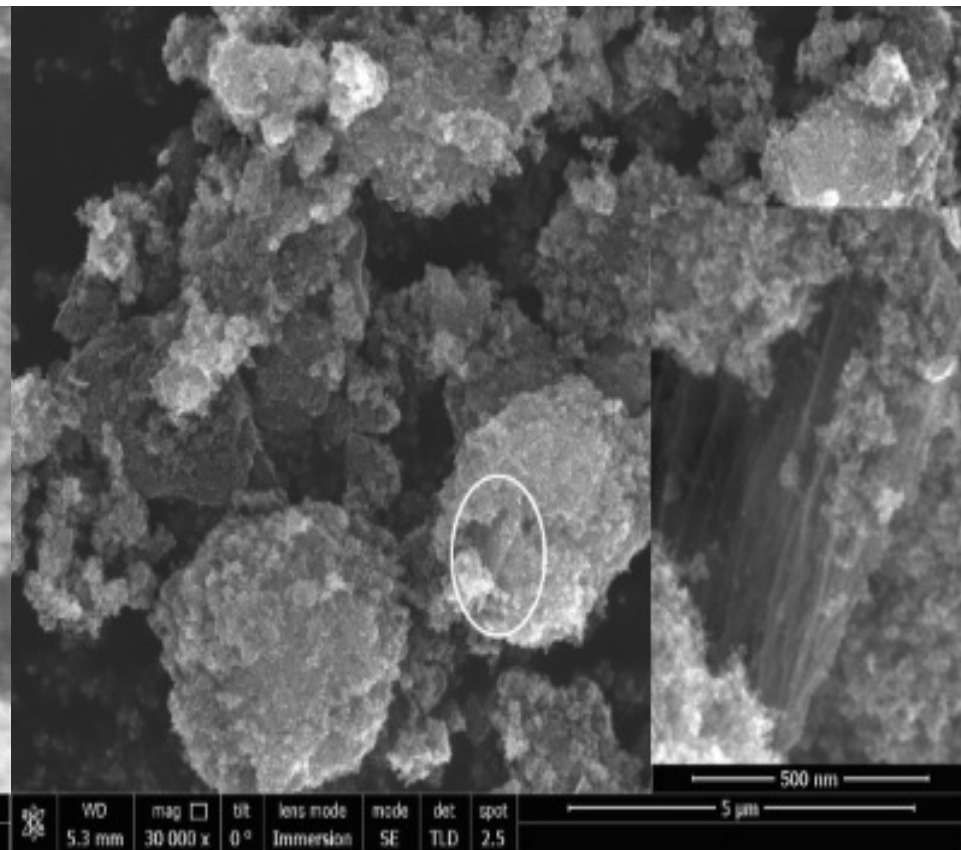
First heating up to 800°C



Thermogram of the secondary heating of the nanodiamond powder up to 1500 ° C with the rate 10 K / min 1 - TG curve, 2 - DSC curve.



a)



b)

Microstructure of the sample detonation nanodiamond after the secondary heat treatment up to the temperature 1500 °C with the rate 2 K/min and the isothermal holding 15 min.

Conclusions

- It is shown that the thermal stability of the detonation nanodiamond is higher than 1500 °C.
- The analysis of the literary data has showed a wide range of the temperature beginning graphitization of the nanodiamond powder. Nevertheless, according to our results the basic process of graphitization the nanodiamond powder occurs above 800 °C. However, after heating of the sample the content of the diamond phase decreased. This is due to the transition of the diamond to the amorphous state.
- After the heat treatment the linear dimensions of the particles powder has increased. However, the dependence of the limit stability of the nanodiamonds from the physical properties of the particles requires the further investigation.



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Thank you for attention...
Obrigado pela sua atenção...



ОБЪЕДИНЕННЫЙ
ИВТЛН





Рис. 7. Сферы применения НА.

Указаны современные (утолщенные стрелки) и разрабатываемые (тонкие стрелки) направления.