

CORRELATIVE ESTIMATION OF STRUCTURE AND COMPOSITION IN THE FORMATION OF CNM SORPTION AND OXIDATION PROPERTIES

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Introduction

Carbon nanostructural materials (CNM) have scientific and innovative interest in materials science of constructional and functional materials. Theoretical and methodological aspects of informational factors studying have conceptual and cognitive character. These factors have some influence on sorption and oxidation properties of CNM.

There is an opinion that physicochemical properties of CNM correlates with their structure only [1]. That's the matter of these questions actuality.

The purpose of this work is to appreciate significance of componential control of impurities in CNM during studying of oxidation and sorption properties of samples without structural change of carbon matrix (CM).

Classification characteristics of CNM as nanostructural systems (NSS) have been discussed in development of Danzer-Than-Molch [2] representations in current work.

The informational-methodological estimation has been offered for "triad": composition – structure – properties of CNM.

An example of theoretic-methodological analysis have been offered for material system (MS) of CNM.

Information on CNM classification

CNM as NSS belongs to the third level of MS hierarchy (from 5 nm to 1000 μm). This level follows cluster level (0.5–5.0 nm) [1].

Carbon macromolecules (nanooions, graphite nanopackets [3], graphite nanofibers, carbon nanotubes, etc.) are base units (BU) of CNM NSS.

Free surface of CNM is limited mainly to an interface "a solid body – gas" [1].

CNM BU can be attributed to granular-fibril type [1]. BU can have various character of arrangement in space [1].

Informational estimation of CNM free surface energy. Specific surface of CNM and graphite is equal to 130 and 8.6 m^2/g correspondingly [4]. High-temperature fibrous materials ACFM have $S_{\text{sp.tot.}} = 50\text{--}800 \text{ m}^2/\text{g}$ [5]. Molar free surface in this case will amount to 600–9600 m^2/g . Average contribution of free energy for metals and high-melting carbides is equal to 1–3 J/m^2 [1]. Average contribu-

tion to total energy of CNM MS can be equal to 1.2–19.2 kJ/mol . These values come near to enthalpy of melting for many metals.

Size factor (according to Gleiter H. [1]) can cause unusual physical and physicochemical properties of CNM.

Discussion

Fundamental materials science CNM "triad" is in many respects declarative abstraction without concrete characteristics of composition, structure and properties.

Transformation of these concepts to self-sufficient informational representation (IR) has concrete character. Nanostructural state of CNM MS should be separated from concept of structure. Hence "triad" can be transformed to "quartet" of representations:

- 1) componential representation (CIR) of CNM composition;
- 2) dynamical representation (DIR) of physical and physicochemical properties;
- 3) structural representation (SIR) of CNM BU;
- 4) local-distributive representation (LDIR) of components and BU. This representation form CNM properties by an establishment of stable connection between CIR and DIR. LDIR characterizes CNM MS as NSS.

CIR, DIR, SIR and LDIR are combined by the relationship of cause and effect. They are parted with quality barrier and relative informational indeterminacy.

These four IR describes CNM as whole MS.

Each IR has its own origins of information (methods, procedures, equipment).

The level of informational indeterminacy and volumes of useful and surplus information grow in series:

$$\text{CIR} < \text{DIR} < \text{LDIR} < \text{SIR} \quad (1).$$

Low information density of CIR methods does not guess existence of CNM structure. The high resolution of LDIR and SIR equipment cannot establish concrete composition of samples.

As the result it is distinctions of observed properties. Lack of information on componential composition of CNM is the reason.

Sorption of xenon has been investigated in temperature dependence during vacuum reduction extraction (VRE) of CNM [7].

It was determined, that carboxyl groups on CNM surface block sorption of xenon. Decomposition products of these carboxyl groups by VRE are gaseous CH_4 , CO , CO_2 and H_2 . It was concluded, that VRE raises specific surface of CNM and sorptive capacity of xenon [7]. However it is possible to make another conclusion on the basis of these important experiment data. Sorption of xenon grows depending on purification efficiency of CNM surface while this surface is constant.

Presence of an organic functional overlying stratum on a surface of CM of other origin was revealed earlier [6]. These facts specify necessity of content control of O, N, H, S in CNM.

Forecasting of CNM oxidation regularities (example)

The purpose of forecasting is to determine properties and characteristics which depend only on structural features of CM (standard state).

The correlation of an inequality of "quartet" (1) has been utilized.

CNM oxidation properties $(\Sigma(\text{DIR})_i)$ without structural change $(\Sigma(\text{SIR})_i = \text{Const})$ are a package of multipleparameter functions of impurities composition $(\Sigma(\text{CIR})_i)$ and their local distribution in CNM $(\Sigma(\text{LDIR})_i)$.

Extraction of impurities will increase a mass fraction of carbon $\chi_C \rightarrow 100\%$ (mass), composition of a matrix will be constant $(\Sigma(\text{CIR})_i = \text{Const})$. Local distribution of carbon will be equivalent to its distribution in BU: $\Sigma(\text{LDIR})_i \sim \Sigma(\text{CIR})_i$.

Oxidation properties will reflect integrated statistical composition of BU: $\text{CNM} = \Sigma(\text{CNF})_i$, $\Sigma(\text{DIR})_{i[\text{OX}]} \sim \Sigma(\text{CNF})_i$. If $i = 1$, $\text{DIR}_{[\text{OX}]} = \text{CNF}$.

Phenomenon of temperature discreteness of the RED/OX identity of CNF

Discrete temperature RED/OX identity of CNF is phenomenon which determines the temperature of concrete carbon BU oxidation [8]. Carbon quantity which has burned at certain temperatures, is proportional to BU mass fraction χ_C in CNM. $\Sigma\chi_{Ci} = 100\%$ (mass) or $\Sigma q_i = 1$ (relative mass parts).

Free total surface of CNM, $S_{\text{sp.tot}}$, will be equal to the total of partial contributions of free CNF surfaces:

$$S_{\text{sp.tot}} \leq \Sigma S_i q_i,$$

where $\Sigma q_i = 1$ – the total of partial mass parts of CNF in CNM (relative mass parts);

S_i – specific surface of CNF_{*i*}.

At $i = 1$; $q_i = 1$; $S_{\text{sp.tot}} = S_{\text{CNFi}}$.

These data are standard characteristic for CNM and a starting information package for the subsequent forecasting its properties.

Conclusions

Comparison of CNM sorption characteristics in a standard and new state will allow to estimate the integrated statistical contribution of local distribution of matrix BU free surface, activating agents and impurities to formation of new CNM properties.

Constant analytical support of researches and technologies allows to estimate features of the physicochemical properties of CNM samples and also materials on their basis.

Results of practical realization of the given model are submitted in the report «Regularities of nanoforms oxidation in carbon matrix» included in the program of the present conference.

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