
COMBUSTION
AND EXPLOSION

Molecular Structural Nonuniformity of Ultradispersed Diamond-Containing Material and the Reasons Why It Arises

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Abstract—An analysis of IR spectra, Raman spectra, and X-ray diffraction intensity curves for diamond-containing materials obtained by the detonation method under different conditions and purified by different methods was used to examine the structural nonuniformity of diamond-containing particles and the reasons why it arises.

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INTRODUCTION

Nonequilibrium manifests itself through fluctuations in various physicochemical parameters, especially energy, and, therefore, the meaning of functions of state becomes uncertain. The concept of local thermodynamic equilibrium, normally used in treating systems with a moderate intensity of fluctuations, is hardly applicable to processes occurring in detonation waves. Thus, it is interesting to gain insights into how nonequilibrium energy distribution affects the condensation of substances under such conditions. The formation of crystals seems to be unlikely, since equilibrium conditions are required for it to occur.

The detonation of high explosives is characterized by a significant degree of nonequilibrium. The detonation of explosives with negative oxygen balance synthesizes an ultradispersed diamond-containing material (UDDCM) [1, 2]. UDDCM is formed under highly nonequilibrium physicochemical conditions [2, 3].

High-intensity short-pulse synchrotron radiation with broad energy spectrum makes it possible to study detonation processes and the kinetic of UDDCM formation in real time [2, 3]. The advantages of this method over other techniques are self-evident. Note, however, that small-angle X-ray scattering (SAXS), employed in [2, 3] (arises due to significant density gradients), may be caused not only by condensation. Alternatively, nonequilibrium chemical processes may be accompanied by interactions of density and energy fluctuations and, consequently by dynamic density variations in the detection zone. Information on the molecular environment of UDDCM particles may prove useful for understanding chemical detonation processes [4–8].

The aim of the present work was to study the structural and kinetic characteristics of an UDDCM particle as an object formed under nonequilibrium thermodynamic conditions.

STRUCTURAL ASPECTS

The available data, partly contradictory, have given rise to different approaches and terminology for describing the UDDCM structural unit.

Admixture molecular groups account for 10–20% of the UDDCM mass, an observation that needs a thorough chemical examination. The mass fraction of carbon in UDDCM samples varies from 95% [9] to 78% [10, p. 698]. It is unlikely that a single substance could manifest such a scatter in characteristics. The morphology of UDDCMs varies significantly, featuring bulbous and X-ray amorphous structures (which also has not yet been isolated). This means that UDDCM is structurally nonuniform, and, therefore, it is reasonable to introduce the notion of a diamond-containing particle (DCP), as the principal structural unit of UDDCM.

Traditionally, an UDDCM particle has been viewed as being composed of a diamond core coated with admixture molecular groups (functional coating). To alleviate doubts over not only surface nature of admixtures [11], it was assumed that they form structures with a developed surface (special clusters or porous aggregates) [12] or that nanosized diamond grains can be thought of as a special type of ultradispersed substances with properties different from those of bulk diamonds.

Along with reflections typical of diamond, X-ray diffraction intensity curves for some UDDCM samples

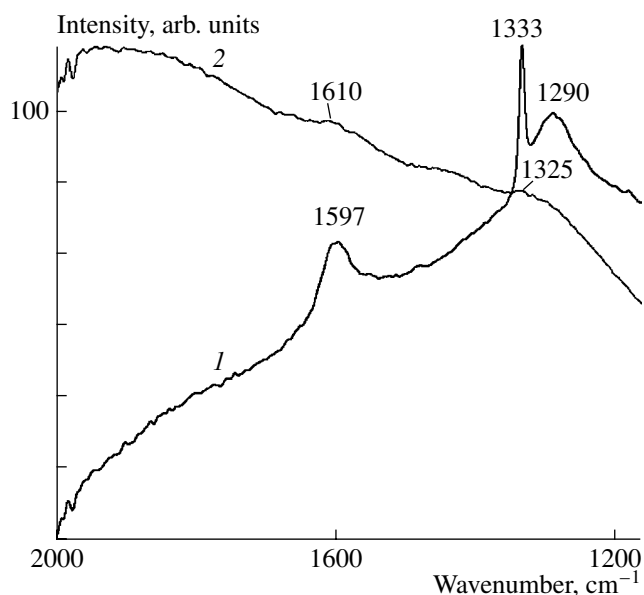


Fig. 1. Raman spectra of UDDCMs synthesized from mixtures of various high explosives: (1) trinitrophenol-hexogen and (2) hexogen-ASM synthetic diamond over the spectral range 500–2000 cm^{-1} .

exhibited unusual reflections at 17° – 19° , which were attributed to molecular groups [10].

In Raman spectra of UDDCM, the characteristic mode of the diamond crystal lattice [13] at 1333 cm^{-1} was found to be nonpredominant [14].

UDDCM possess a number of other specific properties: the density of some samples is as high as 2.8 – 3.0 g/cm^3 (the density of bulk diamond is $\sim 3.5 \text{ g/cm}^3$), admixture molecular groups exhibit high stability, and there exist a double aggregation system and a stable primary structure. Sedimentation investigations showed that the size of this structure lies within 20 – 60 nm [12] or 30 – 50 nm [10]; on the other hand, light scattering measurements yielded 100 nm [4, 6, 7]. These methods detected no finer fractions. Thus, the fact that UDDCMs feature a large number of nondiamond properties calls for a refinement of the notion of its structural unit.

EXPERIMENTAL

Figure 1 displays backward scattering Raman spectra of a UDDCM sample recorded on a Bruker RFS100/S Fourier spectrometer within 100 – 4000 cm^{-1} at a resolution of 1 cm^{-1} . The excitation source was a Coherent Compass 1064-1500N Nd:YAG laser with diode pumping ($1.6 \mu\text{m}$, 800 mW).

Raman spectra make it possible to characterize crystal lattices and molecular structures. The active mode of the diamond crystal lattice is the F_{2g} phonon mode (at 1333 cm^{-1}), while that of the graphite crystal lattice, E_{2g} , features itself at 1575 cm^{-1} ; the A_{1g} phonon mode (1355 cm^{-1}) is typical of finite-size crystals [13].

The spectra shown in Fig. 1 exhibit bands within 1300 – 1320 cm^{-1} , which can be tentatively (based on the previous interpretation) attributed to the diamond structure, and 1600 – 1610 cm^{-1} . Bands with similar positions in UDDCM spectra were observed in other studies, 1630 cm^{-1} [14] and 1620 cm^{-1} [10]. In the review [10], these bands were assigned to the graphite component of UDDCM, while the authors of the experimental work [14] put this interpretation in doubt. It is likely that the 1600-cm^{-1} band is a superposition of several bands. The stretching vibration of the carbonyl group should manifest itself within 1580 – 1900 cm^{-1} . This vibration was observed in IR and Raman spectra [15, 16]. Hydroxyl groups have a Raman band at 1590 – 1600 cm^{-1} [13], in agreement with IR data indicative of UDDCM structurally nonuniform particles containing OH groups.

An analysis of the frequencies of the asymmetrical and symmetrical stretching vibrations of the $-\text{NO}_2$ group suggests that the second contribution may come from $\text{X}-\text{NO}_2$ functional groups ($\text{X} = \text{O}, \text{N}$) [15]. The stretching vibrations of the $\text{O}-\text{NO}_2$, $\text{N}-\text{NO}_2$ groups were observed in Raman spectra at 1640 – 1628 and 1285 – 1260 cm^{-1} and at 1570 – 1520 and 1340 – 1320 cm^{-1} , respectively [15]. Another contribution may be associated with $\text{R}-\text{X}-\text{N}=\text{O}$ groups ($\text{X} = \text{O}, \text{C}, \text{N}$) [15].

The above data suggests the Raman bands at 1290 – 1310 cm^{-1} and 1600 – 1620 cm^{-1} may belong to molecular groups. An analysis of IR spectra [4, 6] showed that UDDCM particles can contain such molecular groups.

Thus, the Raman spectra obtained in the present work and in [14] differ significantly from that of pure diamond. Thus, if molecular groups account for a significant fraction of DCPs, the observed specific features of the Raman spectra can be attributed to vibrational modes of such groups.

We studied the IR absorption spectra of UDDCM samples synthesized by detonating a trinitrotoluene-hexogen mixture and purified by different methods:

- (1) thermooxidation in the presence of boron anhydride (UDDCM-1);
- (2) oxidation by hydrochloric acid (UDDCM-2);
- (3) treatment with a sulfuric acid–nitric acid mixture (UDDCM-3);
- (4) oxidation by air oxygen (UDDCM-4);
- (5) treatment with bichromate (UDDCM-5);
- (6) an UDA-G sample purified from metallic technological admixtures.

The IR spectra were recorded within 200 – 4000 cm^{-1} . A portion of initial UDDCM powder, 1 – 3 mg in weight (depending of the type of the sample) was pressed together with KBr into 1-g pellets.

The size of UDDCM particles was measured using Rayleigh light scattering [17]. The Rayleigh formulas are applicable to light scattering on small particles, when the diffraction parameter, $p = 2\pi r/\lambda_0$, λ_0 is the wavelength, and r is the particle radius) is much smaller

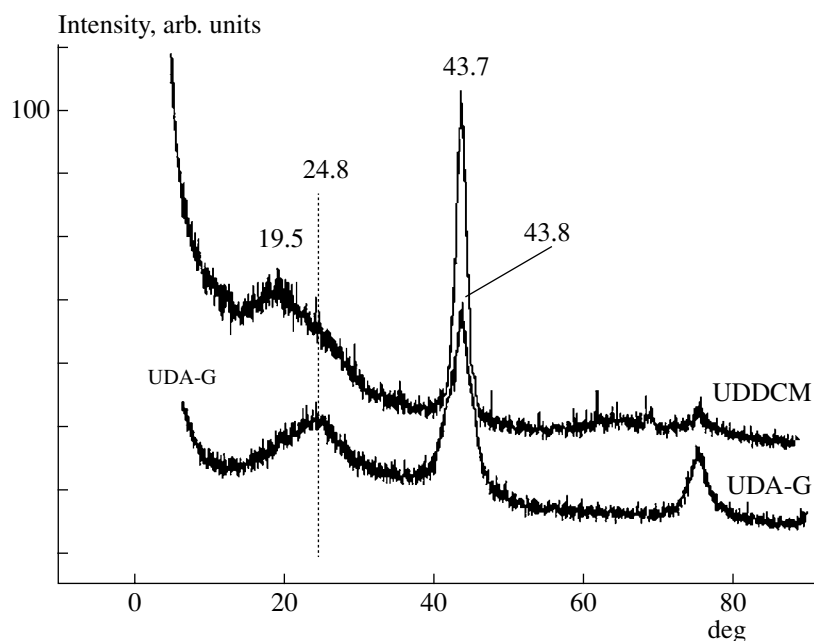


Fig. 2. X-ray diffraction intensity curves for the UDA-G sample and the UDDCM sample synthesized in a molecular nitrogen atmosphere.

than unity. If pm ($m = m_i/m_a$, where m_i and m_a are the refractive indices of the dispersed phase (UDDCM particles) and dispersion medium (KBr pellet), respectively) is much smaller than unity, the optical density in the transparency range is given [17] by

$$2.3D = Nh\pi r^2 \frac{8p^4}{3} \left| \frac{m^2 - 1}{m^2 + 2} \right|^2,$$

where N is the concentration of particles, h is the medium layer thickness, r is the radius of particles, m_i is the refractive index of the disperse phase (UDDCM), m_a is the refractive index of the dispersion medium (matrix), and $p = 2\pi r/\lambda_0$. It is known [10] that diamond-like particles isolated from the detonation products are primary structures with sizes 30–50 nm (in [12], values within 20–60 nm were reported, while experiments on light scattering yielded 100–200 nm [4, 7]), but no finer fractions were observed. This experimental result made it possible to simplify the measurement procedure of this method and decrease the experimental error, since only the relative size of scattering centers was determined [17]. As the transparency range, we used the 2000–2200-cm⁻¹ frequency interval. The digitized spectra were processed using the Microcal Origin 3.5 software.

All the UDDCM samples tested featured the characteristic IR radiation belonging to hydroxyl groups (3400–3500 cm⁻¹ and 1620–1640 cm⁻¹), carbonyl and carboxyl groups (1720–1770 cm⁻¹), and methyl groups (2840–2870 and 2930–2950 cm⁻¹). The specificity of the IR absorption by the different UDDCM samples

over a spectral range of 900 to 1400 cm⁻¹ was discussed in [4, 7].

All the experimental spectra can be divided into two basic groups: the spectra of the samples synthesized in a carbon dioxide atmosphere (in this case, an absorption band at 1260 cm⁻¹ was observed) and those synthesized in molecular nitrogen (with absorption bands of various intensities near 1100–1150 cm⁻¹). The changeover from one buffer medium to another manifests itself through changes in the oxidation temperature and UDDCM yield; therefore, this result is quite expected. The fraction of nitrogen in such samples is normally 2.2–2.3% or more, a observation that makes it possible to divide UDDCMs into two classes. For the samples with a significant optical density at 1100–1150 cm⁻¹, a characteristic feature associated with X-ray reflections at 17°–19° is observed (Fig. 2).

The spectrum of purified detonation products (UDA-G sample) occupies an intermediate position. Thus, although a wide variety of UDDCM samples purchased from different producers was used, it proved impossible to rigorously associate the characteristics of the absorption bands with the methods of isolation and purification of the samples.

As can be seen from Fig. 3, the IR spectrum of UDA-G, a sample not subjected to an intense acid treatment, features, nevertheless, well-pronounced absorption bands belonging to the aforementioned groups. This means that some of the admixtures were present in UDDCM irrespective of which extraction method was used. In other words, some molecular groups are formed before purification during detonation.

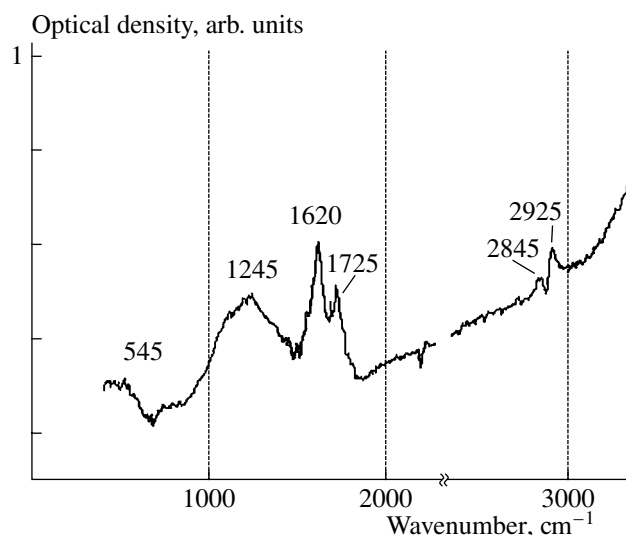


Fig. 3. IR absorption spectrum of the UDA-G sample within 400–4000 cm^{-1} .

Next, we compared the IR spectra of samples isolated by a single method from detonation products obtained in the same explosion chamber but from explosives with different density and composition; i.e., examined how the characteristics of the initial synthesis products affect the IR of UDDCMs. The XRD intensity curves of the samples featured no distinctions. We used explosives with densities of 1.60, 1.67, 1.69, 1.71, 1.72, and 1.73 g/cm^3 . The charges to be detonated were composed of trinitroresorcin (styphnic acid)–hexogen, trinitrobenzene–hexogen, trinitrotoluene–hexogen, and trinitrophenol (picric acid)–hexogen taken in various mass ratios.

Figure 4 compares the IR spectra of UDDCM powders synthesized under identical experimental conditions in the same explosion chamber and buffer medium with the use of a single method of extraction (treatment with hydrochloric acid). The charges were prepared from 70 : 30 (spectrum 1) and 20 : 80 trinitroresorcin–hexogen (spectrum 2) mixtures. The UDDCM sample for which spectrum 1 was recorded contained a larger fraction of trinitroresorcin, and, hence, the fraction of carbon in the initial mixture was higher. The bands belonging to the carbon-containing groups in spectrum 1 (ester (1130 cm^{-1}), carbonyl (1760 cm^{-1}), and to some extent, methyl (2960 cm^{-1}) groups) exhibited higher optical density.

Thus, the larger the content of carbon in the explosive, the higher the optical density of the carbon-containing groups.

The obtained correlation between the elemental composition of the initial explosive and the optical density of the IR absorption bands suggests that a fraction of the functional groups of DCPs, primarily carbon-containing, were formed at high temperatures. In other words, admixtures formed at high temperatures have a

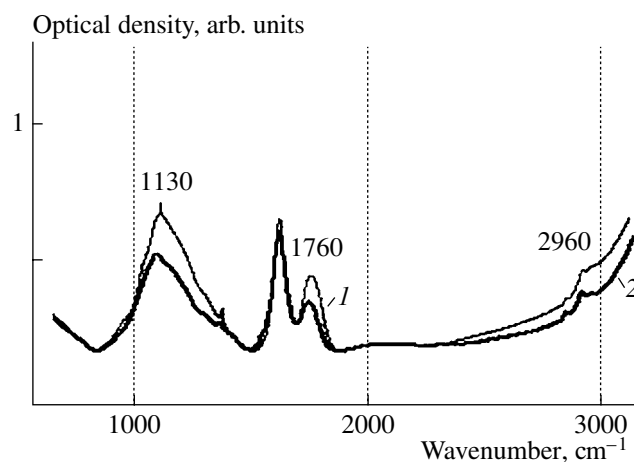


Fig. 4. Comparison of the IR spectra of two UDDCM-2 samples prepared from the detonation products of 20 : 80 (spectrum 1) and 70 : 30 (spectrum 2) trinitroresorcin–hexogen mixtures (in mass fractions).

certain structure accessible for studying by IR spectroscopy, in contrast to surface admixtures, the composition of which is very likely variable.

We treated the UDDCM samples in a low vacuum (10^{-3} Torr) for 90 min at 200, 350, 450, 600, and 900°C and in air at 100, 350, and 700°C for 60 min.

Upon oxidation of UDDCM-1 at 350°C, the 1260- cm^{-1} absorption band, which corresponds to nitrogen substitution defect of type A (two adjacent nitrogen atoms are substituted for carbon atoms in the diamond crystal lattice [4]; i.e., this defect occurs in the core of the diamond-containing grain), was smoothed. At the same temperature, the maximum decrease in the size of scattering centers (by 30%) is observed, as measured by the method described in [17]. Qualitatively, the set of IR absorption bands belonging to the functional groups remained unchanged (Fig. 5). The optical density D of the maxima of the relevant absorption bands was 0.082 (1770 cm^{-1} , 100°C), 0.204 (1630 cm^{-1} , 100°C), 0.083 (1780 cm^{-1} , 350°C), and 0.135 (1625 cm^{-1} , 350°C). The baseline corresponded to the optical density measured at 2000 cm^{-1} .

At 700°C, a temperature higher than the temperature of oxidation of UDDCM, the IR spectrum featured absorption bands within 1000–1150 cm^{-1} (the stretching vibration of the C–O bond) and 1310–1350 cm^{-1} (a band belonging to amorphous carbon inclusions [4]). These absorption bands are directly associated with the oxidation processes. That no type-A absorption bands were observed means that the diamond core had undergone a serious destruction. It is worthwhile to point out that the absorption bands belonging to the functional groups remained stable (Fig. 3). The optical densities of the maxima of the absorption bands belonging to hydroxyl and carbonyl groups were found to be 0.119

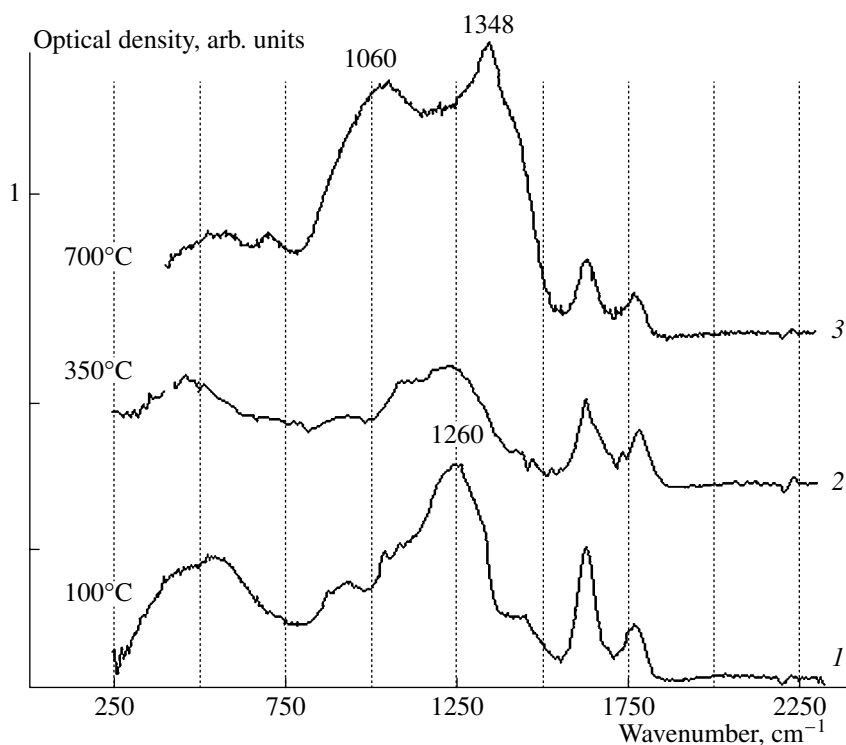


Fig. 5. IR spectra of the UDDCM sample synthesized in a carbon dioxide atmosphere after thermal treatment in air at (1) 100, (2) 350, and (3) 700°C.

and 0.067, respectively. This means that some of these groups cannot be considered as surface ones.

Note that the maximum decrease in the size of scattering centers was about 30%; i.e., the available experimental data do not suggest the primary structure 100–200 nm in size is destroyed. The IR spectra of the samples subjected to thermal treatment in a low vacuum support the conclusion that the admixture functional groups are stable, as do experiments involving irradiation with fast neutrons with energy of $E > 1$ MeV and a fluence of $\Phi = (1.30 \pm 0.19) \times 10^{17}$ neutrons/cm² and with γ -quanta with doses of 0.5 and 183 Mrad. The results of these experiments were examined in [4, 6].

DISCUSSION

Thus, admixtures present in UDDCM can be divided into those formed under high-temperature conditions and secondary ones, which arise during extraction of DCPs from detonation products. These admixtures are likely to be distributed nonuniformly and to have a variable composition. Note, however, that the structure of high-temperature-origin admixtures is stable, and, therefore, they dominate in the IR spectra, determine the character of Raman spectra, and give rise to the specific features of the XRD intensity curves.

The experimental results reported in [4–8, 10, 12] and our studies of Raman and IR spectra upon oxidation and thermal treatment of UDDCM suggest that a

structural unit of a DCP 100–200 nm in size is capable of ensuring the stability of high-temperature-origin molecular groups. In other words, we believe that UDDCMs consist of structurally nonuniform particles 100–200 nm in size. This assumption is consistent with the results of other studies (see, e.g., [11]), where the observation that the number of noncarbon atoms increases upon the oxidative destruction of UDDCM particles (inconsistent with the notions of a single particle with a developed functional coating or an aggregate of such particles) was used to draw conclusions concerning the compositional structure of this material (table).

Indirect evidence that DCPs are structurally nonuniform is a significant scatter in the basic physicochemical characteristics of this material. The elemental composition of UDDCMs (and other properties) varies significantly: from 78 [10] to 95% [9] in carbon (according to [18], 75–90%) and from 10 to 17% in oxygen [10]. The density varies from 2.8 and 3.05 g/cm³ to 3.3 and 3.45 g/cm³. The specific surface area also shows a considerable scatter. UDDCMs can contain bulbous structures and X-ray amorphous phases, information on whether they were isolated is lacking. These experimental observations confirm the conclusion that UDDCMs have a nonuniform structure.

The use of high-resolution TEM made it possible to identify separate objects with sizes as small as 4 nm, although light scattering measurements have not

Dependence of the elemental composition of the UDDCMs extracted from detonation products on the degree of oxidation a [11]

UDDCM samples	Amount of atoms (molecular formula)	Relative (per 100 carbon atoms) content of heteroatoms
Initial sample (UDDCM fraction, 45%; degree of oxidation, $a = 0$)	$C_{100}H_{5.3}N_{2.8}O_{4.1}$	12.2
$a = 26.3\%$	$C_{100}H_{25.4}N_{2.9}O_{22.5}$	50.8
$a = 31.3\%$	$C_{100}H_{34.9}N_{2.9}O_{23.1}$	60.9
$a = 55.0\%$ (UDDCM)	$C_{100}H_{11.2}N_{2.2}O_{9.1}$	22.5
$a = 64.9\%$ (UDDCM)	$C_{100}H_{19.3}N_{2.1}O_{23.5}$	44.9
$a = 74.4\%$ (UDDCM)	$C_{100}H_{18.7}N_{2.0}O_{22.8}$	43.5
$a = 75.6\%$ (UDDCM)	$C_{100}H_{23.7}N_{2.4}O_{22.9}$	48.8

detected macroscopic amounts of such fractions. Note also that DCPs incorporate molecular groups bonds in which are typically covalent. Such groups are known as admixed, since they decrease rather than increase the surface energy. Having a size of 100 nm, DCPs can nominally be considered to be ultradispersed, but it is now clear that the role of the surface and surface groups was seriously overestimated in the previous works. For example, most of the gas release, which was earlier attributed to an active surface, can be accounted for by the UDDCM being nonuniform.

Prerequisites for the Formation of a Structurally Nonuniform UDDCM Particle

The DCP structure we obtained makes it possible to avoid using the phase diagram for carbon or one of its versions for nonequilibrium and ultradispersed systems (the product can be considered as organic or composite rather than carbonaceous). There is another aspect that renders the notion of a phase insufficiently effective. Ignoring the structural factor, we can argue that the characteristics of the synthesis of UDDCM improve with increasing density of the initial explosive. Indeed, an analysis of the available experimental results suggests that the limitations on the synthesis of UDDCMs are associated with the impossibility to produce denser explosives.

Moreover, the authors of [2], a work devoted to the synthesis of UDDCM, did not present the carbon phase diagram, an omission indicative of significant contradictions between the experimental data obtained and their treatment within the framework of the equilibrium approach.

The formation of UDDCMs involves high-temperature nonequilibrium processes [1–3]; therefore, these experiments are more important than those described in [19], which cannot be considered optimal from the point of view of UDDCM preservation. The authors of [20] concluded that C–H bonds are predominantly broken in shock and detonation waves. Note that the same data provide insights into how the conjugation system affects the destruction of various classes of organic compounds.

On the whole, the physicochemical processes in the reaction zone of the detonation wave have been studied insufficiently [21–23]. Direct experimental data raise the questions about the structure of the detonation wave [24] and the nature of the processes occurring in it [23]. Given this complexity, we were forced to employ only qualitative notions of the formation of UDDCMs under nonequilibrium conditions in the reaction zone and, partly, outside it.

It is likely that nonequilibrium manifests itself largely through a sharp increase in the entropy, a behavior that makes the notion of thermodynamic equilibrium be of limited use. In other words, it is reasonable to assume that the main factor responsible for the formation of UDDCMs is nonequilibrium or a sharp increase in the entropy.

By definition, in a nonequilibrium system, processes leading to an increase in the entropy should occur. Any molecular system is characterized by the energies of the rotational, vibrational, and electronic degrees of freedom. An increase in the entropy reflects an increase in the number of states of the molecular system. It is known that the number of vibrations in polyatomic molecules is equal to the number of vibrational degrees of freedom. Therefore, one can expect that nonequilibrium energy will initiate a partial destruction of molecules and, for example, transitions from one-dimensional molecules to two- and three-dimensional structures. The stability of these new three- or two-dimensional structures, by itself, produces no effect on the nonequilibrium process, but the aforementioned tendency in the behavior of the entropy manifests itself, as follows from experimental data on the effect of shock waves on organic molecules [22]. These experiments are indicative of transition to structures with larger dimension. Moreover, as pointed out in the review [21], the nonequilibrium destruction of aromatic molecules differs from the equilibrium one, in agreement with the above tendency. This is in line with ideas put forward in [25].

In our case, under nonequilibrium conditions of synthesis of UDDCMs, this means that molecules of high explosives, as well as additives, become active due to the destruction of the conjugation system. One of the stages of UDDCM formation involves the activation of the carbon atoms of the benzene ring in the explosive molecule. This discussion is indicative of the possibility of the formation of bulk carbon or carbon with a tet-

rahedral (bulk) hybridization of electron orbitals. Such hybridization occurs in diamond-like compounds, while two-dimensional or trigonal hybridization is characteristic of graphite-like structures.

If the nonequilibrium energy of the molecular system is higher than the energy of its electronic states, the initial molecule either decomposes or undergoes substantial reconstruction. As a result, a nonequilibrium energy distribution or energy fluctuations in the decomposition products arise, which in turn gives rise to a nonequilibrium density distribution or density fluctuations.

Fluctuations of electron density are observable through SAXS measurements on detonation products. The above arguments suggest that the significant time of rise of the signal (1–2 μ s) is due to the influence of chemical activity, which, being stronger outside the reaction zone, produces a dynamic contribution to the SAXS signal. The SAXS experiments were based on the relationship between UDDCM formation and density fluctuations (dynamic compressions and rarefactions). The model ACP we constructed consists of a dense sp^3 carbon core and molecular fragments with a lower density. This density profile in the ACP can be tentatively attributed to the effect of fluctuations.

As an extension of the concept underlying the SAXS experiments, we supposed that there is a relation between the stability of molecular admixtures and the chemical processes in the detonation wave. Of such chemical processes, it is worthwhile to mention oxidation and a number of processes involving nitrogen. We identified two types of nitrogen-containing admixtures. Oxygen- and nitrogen-containing functional groups can occur on the surface or in between carbon cores. Type A nitrogen defects do not occur at the surface; i.e., when the characteristics of density fluctuations and the DCP structure are related, processes involving nitrogen-containing compounds can be considered as one of the factors that give rise to fluctuations. The authors of [4–8] put forward the assumption that molecular nitrogen affects UDDCM formation, which, however, needs some refinements. The nitrogen molecule is stabler than CO_2 , and, therefore, its formation is characterized by a significant energy release. The subsequent destruction of this molecule may be accompanied by energy consumption and the formation of type A nitrogen defects.

In principle, UDDCM may contain various elements (oxygen, nitrogen, and hydrogen). Under equilibrium conditions, the system tends to its energy minimum (stability) and, therefore, UDDCMs with a high content of heteroatoms decompose in secondary processes. At the same time, structures containing large amounts of bulk carbon rearrange to form relatively stable diamond-like structures.

Thus, we supposed that nonequilibrium conditions typical of the detonation wave reaction zone give rise to significant density fluctuations (with a compression

region characteristic size of a few to tens of nanometers), which, when a large concentration of carbon is present, may transform into condensed diamond-like forms.

CONCLUSIONS

(1) Experimental IR absorption spectra of various UDDCM samples suggest that the buffer medium in which the synthesis is performed plays a key role. It was suggested to separate these samples into two classes. This result suggests that some molecules and fragments are formed, not during their isolation, as has previously been believed, but under high-temperature conditions in the detonation wave.

(2) A comparison of measured IR and Raman spectra of UDDCM samples revealed some common spectral features. Given a significant scatter in the basic physicochemical characteristics of UDDCMs, we concluded that DCPs 100 nm in size are structurally nonuniform. The main reason why this material is structurally nonuniform is the effect of fluctuations on its formation.

(3) We proposed a new qualitative approach to elucidating the mechanism of the decomposition of molecules of high explosives (used for synthesis of UDDCMs), a process accompanied by the release of conjugation energy and chemical activation in the reaction zone of the detonation wave. The formation of molecular nitrogen and significant energy release are consequences of such activation. The destruction of nitrogen molecules and formation of type-A nitrogen defects are interrelated, a feature indicative of the existence of a stable endothermic process in the reaction zone of the detonation wave. Thus, high explosives can be prepared only from nitrogen-containing compounds with a developed conjugation system.

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