Analysis of the physical properties, composition and structure of soot particles

V A Likhanov¹,4, O P Lopatin¹, A S Yurlov¹ A G Terentiev² and R V Andreev³

¹Department of thermal engines, automobiles and tractors, Vyatka State Agrotechnological University, 133, October prospect, Kirov, 610017, Russian Federation
²Department of Mechanization, Electrification and Automation of Agricultural Production, Chuvash State Agrarian University, 29, K. Marx Street, Cheboksary, 428003, Russian Federation
³Department of Technical Service, Chuvash State Agrarian University, 29, K. Marx Street, Cheboksary, 428003, Russian Federation

4E-mail: lihanov.va@mail.ru

Abstract. A soot particle consisting of crystallites representing several parallel layers of densely packed hexagons with carbon atoms located at the vertices is considered. Such a crystallite structure is similar to a graphite crystal lattice, but less ordered with large distances between the layers, where individual layers can be arbitrarily rotated relative to each other and relative to their common normal. It is shown that the core of a particle with a high salt content of exhaust gases (EG) of a diesel internal combustion engine (DICE) is discharged more, which allows us to distinguish models of the structure of a spherical nanoscale particle.

1. Introduction
Soot is unburned carbon in a DICE. Dissociation, or decay, of particles occurs when the decay forces due to an increase in the vibrational movements of atoms with an increase in temperature begin to prevail over the dissociation forces of a given molecular structure, expressed in the binding energy. Naturally, the process begins with individual molecules that either have the least strong bonds or are activated, and their properties can differ significantly when sampling at different sites of the same flame. During the oxidation of hydrocarbons, there are thresholds of thermal stability for some hydrocarbons, since there are not initial hydrocarbons, but their products, although primary, but nevertheless essential for the oxidation of decomposition [1-7].

2. Methodology
The specific surface area of soot can vary from 15 to 120 m²/g, depending on the technological parameters of obtaining carbon black. Soot consists of 94-99% carbon, chemically bound hydrogen (0.5-3.0%), a certain amount of oxygen and ash elements. At different stages, the atomic ratio of C/H varies from 3 to 15 [8-13].

With the help of electron microscopy and X-ray diffraction studies, it became possible to analyze the morphology of soot particles. The smallest particle is a complex cluster-like formation of carbon globules connected by common carbon layers (figure 1).
The average arithmetic diameter of the primary soot particles (globules) during combustion in DICE of various fuels is from 20 to 90 nm. According to some reports, the size of the primary soot particles can vary from 15 to 170 nm [14-19]. The primary particle is close to a spherical shape, while the aggregates have a complex shape (figure 2).

![Primary particles (globules)](primary_particlessm.png)

**Figure 1.** Primary node diagram.

The structure of the crystal lattice of soot differs significantly from the structure of the crystal lattice of coals. The crystal lattice of coals is ordered, while most varieties of soot do not have an ordered crystal lattice. According to the structure, only the crystal lattice of graphitized soot approaches the lattice of natural fuel. Many authors [20-26] depict the crystal lattice of graphitized soot in the form of a polyhedron, the surface of which is composed of crystallites with basic planes parallel to each other. It is established that the particle consists of crystallites, which represent several parallel layers of densely packed hexagons, in the vertices of which carbon atoms are located (figure 3).

3. Results and Discussion

Such a crystallite structure is similar to the graphite crystal lattice, but less ordered, with large distances between the layers. Individual layers can be arbitrarily rotated relative to each other and relative to their common normal [27-34].

![Images of primary aggregates of soot particles obtained using an electron microscope.]( primary_aggregates.png)

**Figure 2.** Images of primary aggregates of soot particles obtained using an electron microscope.

Elementary crystallites contain from 100 to 200 carbon atoms. The crystallites, consisting of 2-10 plates, have a thickness of 1.2-3.0 nm. A spherical particle with a diameter of 20-30 nm contains 103-104 crystallites. When thermal exposure to soot at temperatures above 1000°C, elementary crystallites
increase in diameter and height. At temperatures above 2800°C, the graphitization process begins, which leads to the ordering of the crystal lattice [35-40].

Figure 3. Structure of crystallites of soot particles.

Depending on the conditions of soot formation, the mutual orientation of the crystallites in the particle may vary. In a particle with a high soot content of DICE EG, the core is discharged more. In this regard, models of the structure of a spherical nanoscale particle can be distinguished [41-43]. A soot particle with a compacted shell consisting of oriented crystallites 1 and a less dense core is shown in figure 4, a.

Figure 4. Models of the structure of a nanoscale particle of diesel soot. 1 - oriented crystallites; 2 – filler; 3 - mineral component.

The orientation of the crystallites on the surface may be disturbed and contain fillers 2 of the mineral components (figure 4, b). A model of the structure is known with a chaotic arrangement of crystallites and in the core containing fillers from mineral components 3 (figure 4, c), stabilizing the position of the crystallites corresponding to the moment of their formation, with a disturbed orientation of the crystallites on the surface. In [44], a model of defective clusters – fullerenes, which are the germ of a particle, is proposed (figure 5) [45-46].
4. Conclusion
Surface growth occurs both on individual spheroidal particles and on aggregates. Diesel soot is prone to the formation of conglomerates containing from several hundred to several thousand spherical nanoscale particles. In the EG of a DICE, soot is an irregular formation with linear dimensions up to 100 microns.

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