THE LAW OF DIAMOND CRYSTALLOGENESIS.

Volodymyr Kaplunenko
"Nanomaterials and Nanotechnologies Ltd",
Ukraine
e-mail: kaplunenkov@gmail.com

Mykola Kosinov
"Nanomaterials and Nanotechnologies Ltd",
Ukraine
e-mail: nkosinov@ukr.net

Abstract. *In our work [19], we presented the law of diamond crystallogenesis applicable to the synthesis of natural and laboratory-produced diamonds. Here, we describe the law of diamond crystallogenesis in more detail. The law of diamond crystallogenesis shows that the rate of diamond growth depends on the number of electrons involved in the synthesis and the oxidation state of carbon in the precursor. Pressure and temperature play a supporting role and are triggers that initiate the electronic mechanism of diamond synthesis. A key aspect of the law of diamond crystallogenesis is electrons, which are considered the most important catalysts in the process of diamond formation, playing a fundamental role in changing the reactivity of carbon and forming the diamond structure. The discovery of the law of diamond crystallogenesis dispels the myth of millions and billions of years required for diamond formation, as well as the myth of pressure and temperature as direct factors in diamond formation. The law of diamond crystallogenesis opens the way to breakthrough technologies for the ultra-fast synthesis of artificial diamonds.*

Keywords: *diamond synthesis**,** law of diamond crystallogenesis, electron as a catalyst, oxidation degree concept.*

1. Introduction

The first theoretical justification for diamond synthesis was Leipunskii's work [1], which laid the foundation for diamond synthesis, specifying the pressure and temperature conditions under which diamond is stable. Leipunskii's diagram was refined and improved by Bundy F. P. [2, 3].

Leipunskii's thermodynamic calculations were confirmed by practical experiments in the 1950s and 1960s [4]. A method for producing artificial diamonds, HPHT, was developed. This served as a convincing reason to believe that pressure and temperature are essential conditions for diamond synthesis. Moreover, pressure and temperature began to be considered direct factors in diamond formation.

At the same time, an increasing number of studies are describing new methods of diamond synthesis that do not require high pressures and temperatures [5-11]. In [5, 6], it was shown that diamonds can be synthesized from adamantane solely using an electron beam. This new method for synthesizing nanodiamonds involves exposing adamantane (a hydrocarbon $C_{10}H_{16}$) to an electron beam at low temperatures, which breaks the C–H bonds, forming a diamond lattice. Nanodiamond synthesis occurs in a vacuum and lasts a short time—tens of seconds. This breaks all the rules and traditional understanding of diamond formation and contradicts the predictions given in the Leipunsky and Bundy diagrams. This new method for synthesizing nanodiamonds demonstrates that extreme temperatures and pressures are not required for diamond formation. Only electrons in a vacuum are required to transform adamantane into diamond.

Controversies have also arisen in the concept of natural diamond formation. Increasing geological data indicate the possibility of diamond crystallization outside the P–T stability region of diamond [12]. Diamonds have been discovered in rocks that do not contain high-pressure minerals [13–15]. These discoveries in geology and laboratory synthesis demonstrate the inconsistency of the concept of diamond formation based on extreme pressure and temperature. A paradoxical situation has arisen: on the one hand, we have Leipunsky and Bundy's calculations, confirmed by the HPHT synthesis method, which indicate the need for extreme pressures and temperatures. On the other hand, we have new geological data and new diamond synthesis methods that do not require extreme pressure and temperature and allow diamonds to be produced outside the P-T stability region. This contradiction requires an explanation. To resolve it, we must consider the fact that the HPHT method actually involves pressure and temperature gradients, which are not represented in the Leipunsky and Bundy diagrams. Furthermore, the HPHT method uses electric current to achieve high temperatures. However, what escapes attention is the fact that, in addition to the thermal effect of the electric current, electrons are injected into the diamond formation zone.

2. The prevalence of empirical research in artificial diamond synthesis, rather than the scientific method.

Currently, laboratory diamond synthesis is more of an art than a science. The selection of catalysts for diamond synthesis lacks a rigorous scientific basis, and their preparation recipes must describe all steps in detail to ensure reproducibility. This is typical for catalytic processes. A similar situation has long been known in catalysis [16-18]. Diamond synthesis as a catalytic process is plagued by the same problems. A successful "recipe" must be developed through trial and error, rather than based on a scientific analysis of the processes occurring during synthesis. The statement cited in [18] is entirely applicable to laboratory diamond synthesis: "*it is more like the art of cooking than stoichiometric chemical synthesis.*"

The development of a scientific theory of diamond formation is a pressing issue. This is driven by recent breakthrough discoveries in diamond synthesis methods, described in [5, 6, 7]. This is driven by the contradictions of the modern concept of diamond formation, based on extreme pressure and temperature. Perhaps we won't have to wait long for a quantitative theory of diamond formation that could universally, using a single equation, describe the process of diamond synthesis from various precursors and indicate the parameters that determine the rate of diamond growth. The lack of a scientific theory of diamond formation hinders the development of diamond synthesis technologies. The lack of a scientific theory of diamond formation has given rise to two myths: the myth of millions and billions of years required for diamond formation, and the myth of pressure and temperature as direct factors in diamond formation.

3. Diamond formation obeys a fundamental physical law.

In our work [19], a unified mechanism of diamond crystallogenesis in nature and in laboratory synthesis was presented, which showed that fundamental particles – electrons – participate in the synthesis of diamond together with the carbon contained in the precursor. The electronic mechanism of diamond synthesis demonstrates stable, repeating relationships between physical quantities and regularly recurring states of the material objects involved in the synthesis. This indicates the existence of a physical law of diamond crystallogenesis that can be represented in a rigorous mathematical formulation. The existence of a physical law of diamond crystallogenesis is also confirmed by the fundamental nature of similar physical processes in various diamond synthesis methods and the participation of a fundamental particle—the electron.

The electronic mechanism of diamond crystallogenesis demonstrates that diamond synthesis involves the fundamental Coulomb interaction of electrons with carbon atoms. To derive the physical (physicochemical) law of diamond crystallogenesis, it is necessary to determine which electronic and carbon parameters should be represented in the law of diamond crystallogenesis. Of all the fundamental parameters of the electron (mass ($m_e \approx 9.109 \times 10^{-31}$ kg), electric charge ($e \approx -1.602 \times 10^{-19}$ C), spin (1/2), radius ($r_e \approx 2.818 \times 10^{-15}$ m), it is the electric charge that exerts force. Electric charge can compete with extreme pressure. The Coulomb electrostatic force is many orders of magnitude greater than the mechanical force caused by any arbitrarily high extreme pressure in the HPHT method. Therefore, we chose electric charge as the parameter of the diamond crystallogenesis law.

The fundamental parameters of carbon are the atomic number (6), mass number (about 12 amu for ^{12} C), atomic radius, and electron configuration, which determines the chemical properties of the atom. Four electrons in the outer energy level allow the carbon atom to form four strong covalent bonds, characteristic of diamond. The degree The oxidation state of carbon is a quantitative measure related to the electron configuration. Therefore, we chose the oxidation state of carbon in the precursor as the parameter for the law of diamond crystallogenesis.

To derive the physical law of diamond crystallogenesis, it is necessary to define a physical quantity useful for comparing the efficiency of different diamond synthesis technologies. Such a practical physical quantity should be a quantitative characteristic of the diamond synthesis process. This practical physical quantity is the rate of diamond formation v_D, which has the dimension in the SI system [mol/s].

The rate of diamond formation v_D must be represented as a function that depends on the parameters of the main participants in the diamond formation process. Representing the diamond formation rate v_D as a function of electron and carbon parameters, expressed by a single mathematical formula, leads to the law of diamond crystallogenesis.

4. The law of diamond crystallogenesis.

The law of diamond crystallogenesis is as follows:

$$v_D = \frac{e \bullet M_e}{F \bullet t \bullet (q_C - q_{C\min})}$$

Fig. 1. The law of diamond crystallogenesis. v_D is the rate of diamond formation (mol/s); e is the electron charge; M_e is the number of free electrons participating in the synthesis; F is the Faraday constant; q_C is the oxidation state of carbon; q_{Cmin} is the minimum oxidation state of carbon (-4); t is the time of diamond synthesis.

The law of diamond crystallogenesis shows the dependence of the rate of diamond formation on the number of M_e electrons involved in synthesis, the electron charge, and the oxidation state of carbon q_C in the precursor. The rate of diamond formation is proportional to the number of M_e electrons involved in synthesis and inversely proportional to the difference in carbon oxidation states (q_C - q_{Cmin}).

The physical law of diamond crystallogenesis follows from the mechanism of diamond crystallogenesis, which is based on the interaction of electrons with atomic carbon and the donor-acceptor interaction of C^{-4} carbon atoms with the diamond surface, forming covalent bonds via the donor-acceptor mechanism.

The law of diamond crystallogenesis demonstrates its universality and applicability to all methods of diamond synthesis. It is represented by a simple and elegant mathematical formula. The law of diamond crystallogenesis includes fundamental physical constants that characterize the participants in diamond synthesis. These participants in diamond synthesis are electrons and carbon atoms.

The main player in the mechanism of diamond formation is the electron. It is represented in the formula of the law of diamond crystallogenesis by a fundamental physical constant: the elementary charge "$e = 1.60217663 \times 10^{-19}$ C" and the number of electrons M_e.

This law states that electrons are the primary driving forces in diamond growth, lowering the oxidation state of carbon to C^{-4}, which facilitates the formation of the diamond crystal structure. This is a revolutionary approach to understanding diamond synthesis in both natural and laboratory conditions. It suggests new technologies for ultra-fast diamond production.

A key aspect of the law of diamond crystallogenesis is that it considers electrons to be the most important catalysts in the diamond formation process, playing a fundamental role in the transformation of carbon into its diamond structure. The mechanism of diamond crystallogenesis involves electrons, which change the oxidation state of carbon from higher positive or neutral states to the C^{-4} state required for diamond synthesis. This electronic transformation of carbon's reactivity "involves" the Coulomb interaction in the synthesis mechanism and initiates the diamond synthesis reaction.

Discoveries arising from this law could lead to new technological approaches that could significantly speed up the process of growing diamond crystals, potentially reducing the process of artificial diamond synthesis to a few hours.

The law of diamond crystallogenesis (Fig. 1) includes Faraday's constant ($F = 9.64853321233100184 \times 10^4$ C/mol). This fundamental constant is a physicochemical constant. It links physical and chemical quantities: the electron charge and Avogadro's constant. Faraday's constant is known to be part of the Nernst equation, the Goldmann equation, and Faraday's law of electrolysis. The law of diamond crystallogenesis is a physicochemical law that also includes Faraday's constant.

The law of diamond crystallogenesis points to the key role of the oxidation state of carbon in the precursor q_C. The law of diamond crystallogenesis suggests that the highest rate of diamond formation is achieved using carbon-containing substances in which the degree of carbon oxidation is minimal. This is observed in practice when using methane (CH_4) as a diamond-forming gas.

The inclusion of the oxidation state of carbon in the physical law of diamond crystallogenesis forces us to evaluate its status in chemistry differently. Oxidation states are not considered physical quantities. They are chemical characteristics of substances. Their presence in a physical law is unusual, as oxidation states are typically used in chemistry to describe the reactivity of substances. However, the degree of oxidation of carbon in the precursor q_C is included in the law of diamond crystallogenesis as a parameter together with and on par with the fundamental physical constants.

The history of the oxidation state concept spans approximately 200 years [20–23]. Despite its widespread use in chemistry, oxidation state is considered an auxiliary, conventional quantity with no physical meaning [24–27]. Scientists have long debated the role of oxidation state in chemistry [26, 28–30]. Some authors point to the universality and fundamental nature of oxidation state [31–33]. Pauling famously stated, "*If scientific progress continues, the next generation may have a theory of valence that is sufficiently precise and powerful to allow chemistry to be considered an exact science, on a par with physics*" [31, 32]. We regard oxidation states as a fundamental characteristic of substances that determines their reactivity. The inclusion of the oxidation state of carbon q_C as a parameter in the law of diamond crystallogenesis, together with fundamental physical constants, indicates the fundamental status of the oxidation state.

5. Conclusions

1. Both natural and laboratory diamond synthesis obey a fundamental physical law.

2. The law of diamond crystallogenesis shows that elementary particles – electrons – participate in the synthesis of diamond together with carbon, which is contained in the precursor.

3. Electrons change the oxidation state of carbon, converting the precursor carbon to the lower oxidation state C^{-4}, which is necessary for the diamond synthesis reaction to occur.

4. A key aspect of the law of diamond crystallogenesis is that electrons are considered catalysts in the diamond formation process, playing a fundamental role in changing the reactivity of carbon and in the formation of the diamond structure.

5. Extreme pressure and temperature play a supporting role and act as triggers that initiate the electronic mechanism of diamond synthesis through the baroelectric and thermoelectric effects.

6. The law of diamond crystallogenesis dispels the myth of millions and billions of years required for diamond formation and the myth of pressure and temperature as direct factors in diamond formation.

7. The fundamental Coulomb interaction is realized in diamond synthesis. The strength of the Coulomb interaction is many orders of magnitude greater than the mechanical force caused by any extreme pressure in the HPHT method.

8. The law of diamond crystallogenesis implies that the rate of diamond growth depends on the number of electrons involved in synthesis and the oxidation state of carbon in the precursor.

9. The law of diamond crystallogenesis is expressed mathematically. It relates the rate of diamond formation to the number of electrons involved in synthesis, the electron charge, the Faraday constant, the oxidation state of carbon, and time.

10. The process of diamond formation, previously considered to require extreme conditions, can now be realized under normal conditions via an electron mechanism, paving the way for new ultrafast diamond synthesis technologies.

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