

# Graphite Carbone Structure

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## Abstract

Carbon graphite is a crystalline form of carbon consisting of layers of hexagonal carbon atoms arranged in a two-dimensional “graphene” structure. Graphene layers are stacked on top of each other, forming a three-dimensional structure with a high degree of anisotropy. The carbon atoms within each layer are linked together by strong covalent bonds, creating a strong, stable lattice structure. However, the layers themselves are held together by weak van der Waals forces, enabling them to slide easily over each other. The properties of carbon graphite are highly dependent on the orientation and alignment of the graphene layers. When the layers are aligned parallel to each other, the material exhibits high strength and stiffness along the alignment direction, but is weaker and more flexible in other directions. Carbon graphite is used in a variety of applications where high strength, rigidity and electrical conductivity are required. Some common applications include electrical contacts, electric motor brushes, and as a structural material in aerospace and defense applications. The aim of our work is to describe the structure of graphite, its physical and chemical properties and its applications.

## Keywords

Graphite, Graphene, Hexagonal Structure, Hardness, Rigidity, Electrical Conductivity

## 1. Introduction

The best-known crystalline forms of carbon are diamond and graphite. Carbon fullerene and nanotubes are the most recent. Graphite itself consists of a stack of two-dimensional layers of carbon atoms in a hexagonal lattice. By definition, one of these isolated layers is called graphene.

Graphite exists in two allotropic forms:  $\alpha$  and  $\beta$ , which can be converted into each other by grinding ( $\alpha > \beta$ ) or by heating to 1000°C ( $\beta > \alpha$ ). Graphite  $\alpha$ , which is the most stable, crystallizes in the hexagonal system. Graphite  $\beta$ , which is relatively unstable and crystallizes in the rhombohedral system, is always found mixed with graphite  $\alpha$  and only in very small proportions. Today, our knowledge of this material enables us to distinguish unambiguously between the presence or absence of the  $\beta$  phase in  $\alpha$ -graphite. In contrast, at the beginning of the century, extensive research into the crystalline system of graphite often led to results that could not be reproduced, because the existence of the two varieties of graphite was not yet known.

A new form of carbon was born: graphene, a sheet of graphite of monoatomic thickness. In this material, which captivates physicists, electrons move as if at the speed of light and have zero mass.

The carbon atom has four outer electrons available for chemical bonds. In graphene, each carbon atom is bonded to three others, leaving one electron per atom to move along the crystal lattice [1].

Based on this situation—mobile electrons in a hexagonal planar lattice—theory and experiment show that the electronic properties of graphene are neither those of a metallic conductor nor those of a semiconductor. Among other peculiarities, graphene's electrons behave like relativistic quantum particles, as if they had lost their mass and were moving at the speed of light.

Graphene, an allotropic form of carbon, forms the basic unit of graphite stacks. It could become a promising material for a wide range of applications (electricity, electronics, mechanics, energy storage, aeronautics, automobiles, telecommunications) [2] [3] [4].

In 1854, mineralogist Kenngott showed graphite lamellae to have a hexagonal outline formed by prisms and pyramids, with rhombohedral faces.

Following the discovery of X-rays, the application of this splendid discovery to the study of graphite's crystalline structure began at the turn of the century. One of the first Laüé diagrams of graphite, described by Ewald in 1914, shows clear senar symmetry.

In 1917, Debye and Scherrer applied their method for analyzing crystalline powders to graphite. The diagram, obtained using a copper anticathode, shows 28 distinct lines, 20 of which are attributed to  $K\alpha$  radiation and the remaining 8 to  $K\beta$  radiation. All these lines are interpreted by means of a rhombohedral-type structure.

In parallel, Hull worked on graphite powder like Debye and Scherrer using  $K\alpha_1$  radiation from molybdenum. His photograph shows 18 distinct lines, which

he interprets using a hexagonal mesh with parameters  $a = 247$  pm and  $c = 674$  pm.

In 1924, Hassel and Mark, followed by Bernai, were the first to study graphite using the rotating crystal method. Their research led them to describe graphite as a hexagonal-type atomic stack.

In 1926, Mauguin, using both Laüie's method and that of the rotating crystal, confirmed these results and proposed the crystalline structure of hexagonal graphite or  $\alpha$ , as we know it today.

It wasn't until 1943 that the existence of two allotropic varieties of graphite was demonstrated. Until then, X-rays on graphite powder had very often revealed the presence of additional lines not belonging to the hexagonal system. Lipson and Stokes showed that these lines could be interpreted by means of rhombohedral symmetry and then proposed the structure of  $\beta$ -graphite.

In 2004, Andre Geim's team [1] succeeded in fabricating a two-dimensional crystal. The thinnest crystals previously obtained were at least ten atomic planes thick. Starting with graphite, A. Geim and his colleagues obtained a kind of giant planar molecule, named graphene, formed solely of carbon atoms linked together to form a network of hexagons [1].

## 2. Characteristics of the Crystalline Structure of Graphite

When there is a differentiation between the cohesive energy of interatomic bonds in a crystal along a plane (a, b) and the direction perpendicular (to this plane), the material has a lamellar (or sheet) structure. The layers are linked by relatively weak bonds of the van der Waals, hydrogen or electrostatic type, compared to the bonds in the layer plane, which may be covalent. There is a wide range of lamellar materials, depending on the structure of the sheets and the occupation of the inter-foil spaces. Lamellar materials can be classified according to the number of layers in the laminae or, for example, the electrical charge of individual laminae. From the point of view of electrical charge, there are three types of lamellar materials: sheets can be neutral, cationic or anionic [5] [6]. The classification can also be made according to the number of atomic sublayers in the sheets; this links the flexibility of the sheets to their complexity [7]. According to this latter classification, graphite is made up of two layers, each of which is made up of two sublayers: one layer is made up of an assembly of benzene rings, each with 6 delocalized electrons. The atoms in benzene are generally linked by covalent bonds, and the inter-lamellar distance is often defined as the distance separating the centers of two consecutive layers [8].

Graphite is one of the naturally stable forms of crystalline carbon. Its structure is made up of layers called graphene, within which carbon atoms form hexagonal cells thanks to  $sp^2$  bonds; each atom is covalently bonded to three others, 1.42 Å apart. The interlamellar bond is of the Van der Waals type, resulting in a high interlamellar distance of 3.35 Å. The weakness of van der Waals-type interlamellar bonds compared with covalent bonds between carbon atoms in graphene

planes explains graphite's anisotropic properties and the possibility of particular chemical reactions, notably those leading to the formation of graphite intercalation compounds. These are the result of the intercalation of one or more layers of atoms or molecules of different species between the graphene planes. The lamellar structure is preserved, with varying degrees of modification of the intralaminar distances. The intercalation process leads to expansion along the *c*-axis perpendicular to the planes [9]. The number *n* of carbon planes between two intercalant layers defines the *n*-stage. Generally speaking, the stage is inversely proportional to the intercalant concentration. Graphite sheets have two types of basic arrangement: the ABAB type, where planes A and B are aligned on the *c*-axis; and the ACAC type, where planes A and C are aligned on the *c*-axis.

### 2.1. Mesh Description

The structure is hexagonal with space group  $P6_3mc$ .

The parameters are:  $a = 2.456 \text{ \AA}$  and  $c = 6.696 \text{ \AA}$ .

The reduced atom coordinates are:  $(0, 0, 0)$ ;  $(0, 0, \frac{1}{2})$ ;  $(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$ ;  $(\frac{1}{3}, \frac{2}{3}, \frac{3}{4})$  (Figure 1).

This structure consists of a stack of sheets. Sheets with whole dimensions are of type AB, and those with half-integral dimensions of type AC (Figure 2). There are strong covalent bonds in the lamina plane: each carbon is linked to three other carbons ( $C - C = 1.42 \text{ \AA}$ ). The sheets are linked by Van der Waals forces (the distance between sheets is  $3.35 \text{ \AA}$ ). Conductivity is high in the planes and very low in the perpendicular direction [10] [11] [12] [13] [14].

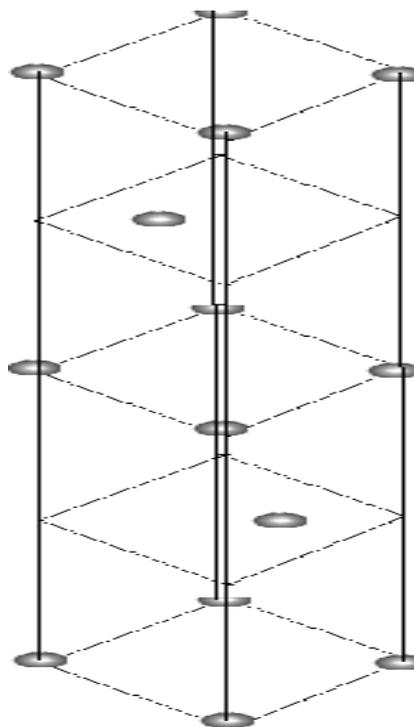
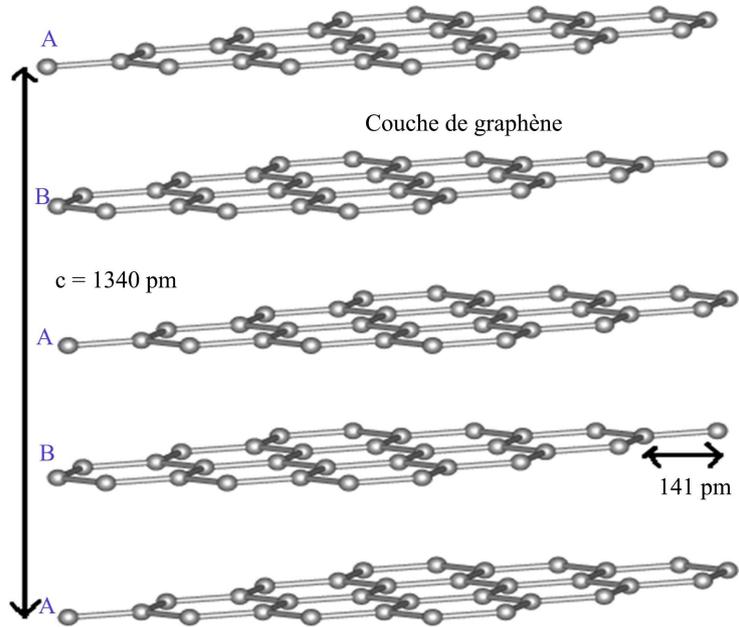


Figure 1. Graphite elemental mesh.



**Figure 2.** Graphite structure.

## 2.2. Mesh Multiplicity

Multiplicity =  $((4 \times 1/12 + 4 \times 1/6)$  mesh vertex +  $(2 \times 1/6 + 2 \times 1/3)$  stop mid-point +  $(1 + 1)$  mesh midpoint).

Graphite multiplicity = 4 carbon atoms per graphite unit cell.

## 2.3. Coordinate

Carbon is trigonal, so the coordinates are 3.

## 2.4. Relationship between Mesh Parameters

In the drawing,  $d = d_{C-C} = 142$  pm.

And  $c = 4 \times d_{A-B} = 4 \times 335 = 1340$  pm.

## 2.5. Compactness

$$C = \frac{\text{Volume of atoms}}{\text{Volume of mesh}} = \frac{4 \frac{4 \times \pi \times r_C^3}{3}}{c(a \wedge b)} = \frac{4 \frac{4 \times \pi \times r_C^3}{3}}{ca^2 \frac{\sqrt{3}}{2}}$$

taking  $r_C = d_{C-C}/2 = 71$  pm gives  $C = 0.256$ . This structure is less compact than diamond carbon.

## 2.6. Mass Density

$$\rho = \frac{\text{mass of atoms}}{\text{mesh volume}} = \frac{4 \frac{M_c}{N_a}}{ca^2 \frac{\sqrt{3}}{2}}$$

*i.e.* with  $M_C = 12$  g/mol; we get:  $\rho = 2300$  kg/m<sup>3</sup>

On the other hand, a density of  $\rho/\rho_{\text{water}} = 2.3$ .

Graphite is therefore slightly less dense than diamond, mainly due to the distance between the sheets, and much less compact. The industrial process used to manufacture synthetic diamond therefore requires high pressures. Graphite is very stable within a single sheet, for the same reasons as for diamond. However, it is brittle perpendicularly to the sheets, as the sheets can slide over one another, a process known as cleavage. This makes it possible to design solid lubricants that are indispensable in conditions where oils would evaporate, such as in space. For each layer, the carbons are trivalent, leaving a delocalized electron. As this electron has no reason to favour one carbon over another, it will be highly mobile, being present “just about everywhere at once”. As a result, light is totally absorbed by these electrons, making graphite an opaque, black compound. What’s more, graphite will be a very good conductor in the plane of the sheets, but the absence of electrons between the sheets makes it insulating parallel to the sheets. This property is used to make graphite electrodes.

### 3. Graphite Applications

Graphite is used for its physical and chemical properties: chemical neutrality, heat resistance, thermal and electrical conductivity, low coefficient of thermal expansion, low coefficient of friction and low X-ray and electron absorption coefficient. All these properties enable graphite to be used in a wide range of industrial sectors for a multitude of applications, such as the manufacture of glass, aluminum, semiconductors and chemicals [15] [16].

The main sector of use for graphite is the refractory industry, with a very wide variety of products ranging from bricks to crucibles; over the last twenty years, two major innovations in the refractory industry have been the introduction and increasingly widespread use of magnesium-carbon bricks in blast furnace linings, and the increasingly frequent use of alumina-graphite refractories for continuous casting.

In foundries, graphite is used as a refractory lining, mixed with a binder (fire-clay, mica, sand, etc.); it prevents the metal from sticking to the mold walls, thus facilitating the demolding of mattes after cooling.

In powder form, graphite is used as a lubricant or as an electrically conductive coating.

The use of graphite in pencil leads is declining.

Graphite is used in anode production for all major battery technologies. Demand for batteries, mainly nickel-metal hydride and lithium-ion batteries, has grown considerably over the past 30 years. This growth has been fuelled in particular by demand for batteries for portable electronic devices, power tools, computers, smartphones and tablets.

Graphite is one of the most important elements in the manufacture of lithium-ion batteries. This technology uses around twice as much graphite as li-

thium carbonate. The emergence of plug-in hybrid and electric vehicles means that more and more lithium-ion batteries need to be manufactured. These batteries incorporate large quantities of graphite (95% graphite in a lithium-ion battery). Electric vehicle batteries should further increase demand for graphite. For example, a lithium-ion battery in an all-electric Nissan Leaf vehicle contains almost 40 kg of graphite.

Foundry mold linings (crucibles and various metal-casting utensils); automotive industry and friction products (e.g. graphite is used in brake and clutch linings, engine parts, electric generators and mechanical seals);

The paint industry (e.g., graphite is used to manufacture anti-corrosive and anti-static paints);

Advanced technologies (e.g., graphite is used as a moderator in nuclear reactors and as a heat-stable substance in the manufacture of rocket components, as well as being used in the manufacture of fuel cells for vehicles);

Many other products, such as industrial lubricants, metal powders, polymer and rubber components, and fire retardants;

The manufacture of lead pencils.

In 2018, worldwide, graphite use in batteries was around 14%, compared with 46% in refractories, 14% in foundry, 6% in friction products, 5% in lubricants, 4% in recarburizers and 2% for textured graphite (Roskill 2019). Battery production is expected to increase and become the main market for graphite by 2027, overtaking the main conventional markets for graphite electrodes and refractories.

Other uses: the main uses for refractories include brake linings (replacing asbestos), electric batteries, brushes and carbons for the electrical industry, etc.

It's a semiconductor. It is used in electrical brushes for motors and other rotating machines.

## 4. Manufacture of Synthetic Graphite

Synthetic graphite is obtained by the graphitization of petroleum coke. The coke is mixed with a coal tar binder and a small quantity of oil is heated and then extruded. The product thus obtained is subjected to a temperature of 800°C to 1000°C to transform the binder into solid coke and allow removal. The coke resulting from this operation is again impregnated with tar or bitumen to reduce its porosity and the graphitization is completed in an electric oven, between 2600°C and 3000°C, which has the effect of graphitizing the carbon in the binder.

### Applications of Synthetic Graphite

Since synthetic graphite has several different properties and characteristics than natural graphite, these two products have separate uses and markets. As a general rule, synthetic graphite is purer and has a lower crystallinity than its natural counterpart: these characteristics make it suitable for the manufacture of electrodes for electric furnaces: this use represents three-quarters of the current

consumption of synthetic graphite.

It is also used as a moderator and reflector in nuclear power plant batteries and, in the form of carbon fibers, it is present in a wide range of products (from aeronautics to tennis rackets).

## 5. Physical and Chemical Properties of Graphite

The multiple uses of graphite arise directly from the physical properties of this mineral, which themselves arise directly from the crystallography of this solid phase in which carbon occurs [17].

**Hardness:** graphite is a very soft body, with a hardness of 1 to 2 on the Mohs hardness scale [17] [18].

**Density:** varies between 2.1 and 2.3 depending on the degree of crystallinity and graphitization [17] [18].

**Resistivity:** is greater than that of copper, even according to the direction along the elementary sheets, the resistivity decreases with the temperature between 500°C and 1000°C, to regain the value it has, at room temperature, between 1500°C and 2000°C [17] [18].

**Lubricating property:** graphite is an excellent lubricant; this property is linked to two factors: the low coherence between the sheets, which slide very easily relative to each other, and the presence of gas absorbed on the surfaces of the sheets. This property is measured by the static friction coefficient  $\mu_s$ , for natural graphite  $\mu_s = 0.15$ , very low value.

**Anisotropic properties:** corresponds to an anisotropy of the mechanical properties (cleavage, plasticity), physical (electrical and thermal conductivities, graphite is conductive in the plane of the sheets; but 200 times less good conductor in the direction perpendicular to the sheets) and chemical (intercalation reactions).

Very friable material: this is explained by the low-intensity bonds which connect the layers and which break easily.

**Its dark color:** It is once again the crystal structure that will dictate how light will behave within an object. Either it is reflected in it, refracted in it or absorbed. Graphite is black because of the large delocalization of electrons in the lattice which causes light to be absorbed there.

**Oxidation resistance:** the rate of oxidation (in air or oxygen) varies depending on the size of the particles and the temperature. Certain impurities increase this rate by catalysis effect:

The reduction in particle size increases the rate of oxidation by increasing the surfaces available for attack by oxygen.

**Temperature:** oxidation is imperceptible at 400°C and very rapid at 850°C. it is an exothermic reaction that is self-sustaining and can quickly get out of control.

### Natural Graphite

It is a mineral composed exclusively of carbon (C) crystal structure and hex-

agonal shape. Its color varies from black to gray-black. It is a soft, flexible mineral, with a metallic luster and a greasy and shiny appearance characterized by:

- A Low density which varies from 2.1 to 2.3;
- A low hardness of 2 on the Mohs scale (scratchable by a fingernail);
- A very high melting point (3500°C).

Graphite is a mineral substance with remarkable properties. In a vacuum, it resists extreme temperatures (2800°C).

Unlike most materials, the mechanical properties of graphite increase with temperature. It is an excellent conductor of electricity and has very good resistance to chemicals, including acids and bases. The crystalline structure of graphite also gives it a very low coefficient of friction. In addition, it is easily machinable.

In the field of very high temperatures, graphite does not have many equivalents. It is one of the only materials that can withstand very high-temperature conditions without damage.

## 6. Conclusion

Graphite is a mineral that is, one of the natural allotropes of carbon. Its structure is made up of non-compact hexagonal sheets; the atoms of carbon are strongly linked by sp<sup>2</sup>-type covalent bonds, while the bonds between the sheets are weak, of the  $\pi$  type, which explains why it presents different chemical and physical properties.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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