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ARTICLE

Discovery of Structural Elements that Form Amorphous Materials

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ABSTRACT

One of the important and unresolved problems of materials science is the structure of amorphous solids. This paper reveals the secret of the structure of amorphous materials through picoscopic visualization of electron orbitals. Picoscopy is a precision experimental method for measuring the thickness of a real electron orbital body in the metric unit picometers. The results of the study of thousands of electron orbitals in amorphous carbon revealed the absence of crystal-forming elements: a) short-range order and b) strong covalent chemical bonds. However, it was found that atoms in amorphous solids are bound by unpaired valence electrons, which form weak interactions due to dipole polarization. Therefore, chemical bonds in amorphous solids are different from those in crystals. Accordingly, the amorphous solids are allotropes. This study shows that unpaired electron interactions form previously unknown polygons with the general formula Cn: a) triangle (C3); b) quadrangle (C4); c) pentagon (C5); d) hexagon (C6). The polygons create the short-range structure of the amorphous solids. It is polygons that are responsible for the universal spatial parameter of the order of ~300 pm, with which the structure of amorphous solids of various natures (semiconductor, dielectric, and metallic) is associated. The unpaired electron interaction and polygons play a fundamental role in the nature of amorphous materials.

Keywords: Amorphous Solids; Polygons in Amorphous Solids; Unpaired Electron; Covalent Bond; Real-Life Electron Orbital

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ARTICLE INFO
Received: 22 March 2025 | Revised: 23 April 2025| Accepted: 4 May 2025 | Published Online: 12 May 2025
DOI: https://doi.org/10.55121/nefm.v4i1.400

CITATION
Kucherov, O.P., Rud, A.D., 2025. Discovery of Structural Elements that Form Amorphous Materials.
New Environmentally-Friendly Materials. 4(1): 48–56. DOI: https://doi.org/10.55121/nefm.v4i1.400

1. Introduction

Amorphous solids represent an important class of new environmentally friendly materials [1]. The first system to attract considerable interest from researchers and practitioners was amorphous selenium, which gained prominence first as a material for photosensors and then in xerography [2]. Recently, the main direction of fundamental and applied research has been the study of amorphous silicon, which has found application in the production of solar cell elements, the cost of which is significantly lower than when using monocrystalline silicon (although the latter has a higher efficiency) [3]. Amorphous metal-silicide resistive alloys have also found practical application [4]. Amorphous carbon occupies an important place in human life. It is anthracite coal, shungite carbon, carbon black coatings, synthetic black carbon, and many others. Amorphous carbon is on the World Health Organization's List of Essential Medicines [5].

From the point of view of fundamental science, the problem of the structure of amorphous solids is considered one of the important and unresolved problems of materials science. How are solids constructed in conditions of chaos with which amorphous solids are usually associated? Answering this question is no easier than answering many fundamental questions of astrophysics and elementary particle physics. Through careful research [6–9], it has been established that the abundance of carbon black has a unique commonality of basis, namely nano-micro-sized molecular compositions of carbon atom structures. It is customary to assume that amorphous solids are systems with predominantly covalent chemical bonding [10], which are characterized by the presence of short-range order (coordinated arrangement of nearest neighbors) in the absence of long-range order, i.e., translational symmetry at the macro level. So far, existing methods do not reveal the fine details of the structure of amorphous solids. Unfortunately, X-ray scattering in amorphous solids does not produce individual peaks, which currently limits analysis and makes it impossible to create a theory for amorphous materials like the well-developed theory of crystals [11].

It turned out that, contrary to the disorder with which their structure is usually associated, for amorphous solids of various natures (semiconductor, dielectric, metallic), there is a universal spatial scale of ~ 1000 pm — an order parameter that can play a significant role for the theory of amorphous solids [12,13]. The spatial heterogeneity of disordered solids leads to the appearance of characteristic features in the vibrational properties, changes the mechanism of relaxation of electronic excitation, and determines the specificity of charge transfer [12,14]. Of all the states of matter, only the crystalline state stands out sharply with its geometric order in the arrangement of atoms at fairly large distances. This has made it possible to achieve significant success in understanding the crystalline state by experimental methods and to create satisfactory theoretical models. However, non-crystalline materials do not have such order if we approach them with "crystalline" standards. An additional problem with amorphous solids is their characteristic local placement of atoms or local allotropic structures [13, 15-17]. Therefore, after more than 50 years of research, an atomic theory of these properties is still missing [18]. The structure of amorphous solids has lost order, and the study of different substances does not reveal any regularities. A large number of studies have found that each substance has its own properties. There is no regularity in their structure, and the only approach is to study each substance and identify its individual features to control its properties. Studies show that the structure of amorphous solids is fundamentally different from that of crystals.

This research aims to reveal the structure and pico-sized formations in amorphous materials by direct visualization of electron orbitals by picoscopy.

2. Technology

Picoscopy is a technology used to capture and store images of real-life electron orbitals. It is a sensitive method for measuring subatomic details of the amorphous materials. The principle of picoscopy is as follows. From quantum mechanics, it is known that the body of an atom consists of an orbital, which is described by Schrödinger's wave function [19]:

$$\psi(\mathrm{x,y,z,t}) = \mathrm{C(x,y,z)\exp\{iEt/h\}}, \qquad (1)$$

where ***E*** is electron energy, ***h*** is Planck's constant, and ***C(x,y,z)*** is amplitude of oscillation. The satisfactory statistical interpretation of $|C(x,y,z)|^2$ as the probability density was first given by M. Born.

As O. Kucherov proved [20], a plane wave of an electron beam, passing through an electron orbital along the line z in accordance with quantum superposition, redistributes its intensity directly proportional to the square of the oscillation amplitude $C(x,y,z)$. As a result, the brightness $J(x,y)$ of the picoscope screen is directly proportional to the thickness of the orbital in the plane x, y.

It is known that the thickness is 100 pm, and at this point x, y on the screen, the intensity reaches a maximum J_{max}. This fact allows the orbital thickness $\Xi(x,y)$ to be expressed in picometers [21]:

$$\Xi(\mathrm{xy}) = \mathrm{J(x,y)} * 100/\mathrm{Jmax(pm)}. \tag{2}$$

The picoscope can measure the thickness in metric units of picometers at each point of the real-life orbital body by equation (2). In contrast to the theoretically calculated wave function $\psi(x,y,z,t)$, in the work [21], it was proposed to call the real-life electron orbital a Ξ-orbital (ksi is a letter of the Greek alphabet). The Ξ-orbital creates both the atom core from the inner electrons and the valence bonds from the outer electrons, i.e., the orbital makes up the entire material world. Therefore, picoscopy creates Ξ-orbital images of real subatomic objects.

Thus, picoscopy is a sensitive method for measuring every detail of the amorphous structure of materials.

3. Experiment

Graphite was milled in an argon gas atmosphere in the laboratory planetary ball mill Fritsch Pulverisette P-6 at room temperature. The rotation speed was 400 rpm for all experiments. The ratio of balls to sample weight was 30:1 [22]. A transmission electron microscopy (TEM) study is performed using the high-resolution microscope JEOL JEM-2100F. Direct images of the Ξ-orbitals of crystalline and amorphous carbon were obtained by equation (2) using the technology described in the work of Kucherov and Rud [23]. The experiment was planned in such a way that both the crystalline and amorphous forms of carbon were depicted in one picture. For this, crystalline carbon in the form of graphite was taken, which was ground in a ball mill. In this case, the crystals gradually lost their strong covalent bonds and passed into an amorphous state.

Direct visualization of amorphous solids with a large volume of picoscopic experiments allows us to see the features of chemical bonds with high resolution and record their shapes and sizes. Picoscopic studies of chemical bonds have shown the existence of previously unknown chemical bonds caused by unpaired electrons [20]. The elongated shape of the Ξ-orbital creates polarization and a weak dipole bond. Visual picoscopic studies have shown that it is the unpaired electrons that form amorphous solids.

As a result of studies using the method of direct visualization of atoms in amorphous solids, the complete absence of both long-range and short-range order was firmly established.

Figure 1 shows the pure form of crystalline carbon (left). Atoms in crystalline graphite form layers with cream-colored covalent chemical bonds of sp^2-hybridization. The Ξ-orbitals have a thickness of 60 pm in yellow color. The green unpaired electrons form the forces that connect the layers together.

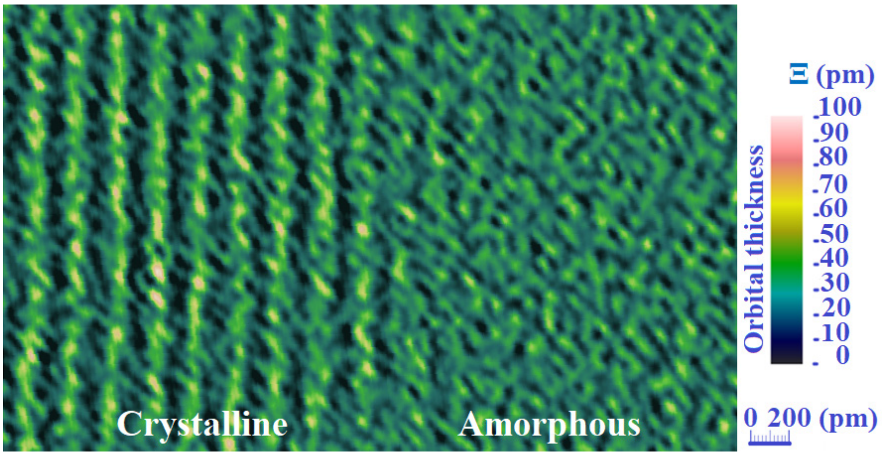

Figure 1. Ξ-Orbitals Image of Crystalline (Left) and Amorphous (Right) Carbon Allotropes, Which Were Obtained on One Sample. Note the Different Chemical Bonds. The Ξ-Orbital Thickness Scale in Picometers is Shown According to the Formula (2) (Right).

Atoms in amorphous solids (right) are bound by weak unpaired electrons, which are created by elongated green-colored Ξ-orbitals, corresponding to a thickness of 30 pm. Sometimes these valence electrons are called almost unpaired [24]. That is, amorphous solids are new, previously unknown materials. They have neither long-range nor short-range order, nor covalent bonds. The amorphous solids are allotropes with zero hybridization. There is no hybridization between atoms in amorphous solids, but they are attracted to each other by weak physical forces. These forces are caused by the elongated orbitals of the unpaired valence electrons, which act through the dipole moment. The amorphous atoms exist in a disordered manner, like a gaseous medium.

4. Electron Configuration of Amorphous Atoms

Studies of Ξ-orbitals by picoscopy show that atoms in amorphous solids do not build a crystal lattice, even at short-range order. As picoscopy shows, atomic Ξ-orbitals have a binary structure and are divided into internal and external. Internal orbitals make up the atomic core [25]; they are closed and ball-shaped. Atomic cores have spherical shapes of pink color. The average thickness of the atomic cores is approximately 100 picometers, as taken into account in the formula (2). Valence electrons create external Ξ-orbitals; they are elongated and chemically active. The thickness of the external electron orbitals is approximately 40 picometers (green color).

Figure 2 shows the binary atomic structure of individual carbon atoms in the amorphous state, consisting of atomic cores and outer valence electrons. The atomic cores have identical spherical shapes in cream and consist of chemically inert electrons. The outer valence electrons are chemically active and have an elongated green shape. Carbon atoms are divided into a core with the electron configuration of helium [He] and four outer valence electrons $2s2p^3$. The space without orbitals has zero intensity (black).

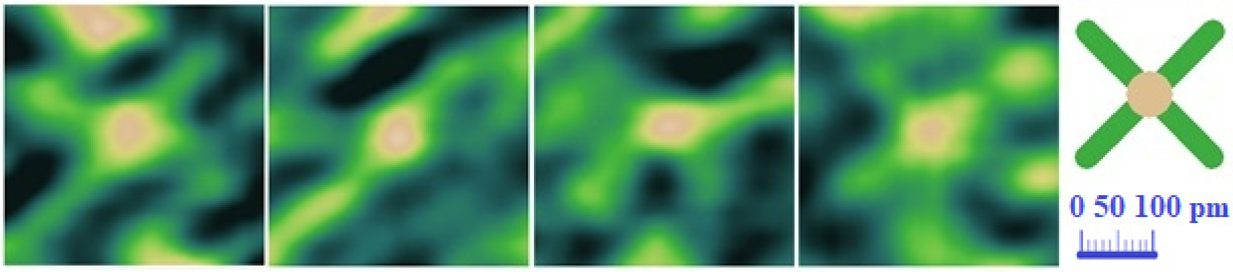

Figure 2. Ξ-Orbital Images of Atomic Cores and Four Outer Electrons for Individual Carbon Atoms in the Amorphous State. The Skeletal Formula of a Tetravalent Carbon Atom is Shown on the Right [26].

5. Unpaired Electron Interaction

In chemistry, it is known that all electrons in an atom are divided into two groups. These are internal electrons, which are chemically inert, and external chemically active valence electrons.

Among the great variety of chemical interactions, there are two strong chemical bonds. Firstly, this is an ionic bond, when a valence electron passes from one atom to another, forming an electron pair of two electrons with opposite spins on the same energy orbital. Secondly, this is a covalent bond, in which two valence electrons located on different atoms create hybridization. Moreover, both electrons must be on the same orbitals, and their spins must be opposite.

In addition to strong chemical bonds, there is a weak van der Waals interaction. **Figure 2** clearly shows that all four valence unpaired electrons rotate in elliptical orbits that correspond to Sommerfeld's quantum mechanical theory [26]. The electric dipole moment of the elliptical orbits creates the van der Waals interaction [19]. The experimentally obtained orbitals correspond to Density Functional Theory calculations [19], namely the Thomas-Fermi model [27]. The charge density increases from the center of the atom, reaches a maximum, and then decreases. In this model, there is no clear limit to the electron density, and the experiment also does not give a clear limit to the disappearance of the charge.

It turned out that all the disorder of the amorphous structure is formed by Coulomb forces created by the elliptical orbits of unpaired electrons. It is the unpaired electrons that are the physical foundations of the formation of structure in amorphous materials. These forces are too weak to create a crystalline structure. The *Ξ*-orbital of the unpaired electron creates a dipole moment and weakly attracts positive charges of the atom nucleus and, thereby, creates an unpaired electron interaction, which is the basis of amorphous solids.

6. Polygons in Amorphous Solids

Picoscopic studies of large volumes of amorphous solids convincingly reveal the nature of formations, which are perceived as short-range order by X-ray scattering methods. Weak molecular bonds are formed in polygons in amorphous solids. They are not stable and, most likely, cannot exist outside the amorphous solids. The polygons do not combine. Therefore, the short-range order extends only to 1-2 atoms, as it seems from previous studies.

Picoscopic studies have shown that it is orbitals of unpaired electrons that determine the geometry of amorphous solids. What is considered short-range order is actually an unstable bond of three, four, five, or six atoms. These are polygons. As shown in **Figure 3**, the general formula is C_n: a) triangle (C_3); b) quadrangle (C_4); c) pentagon (C_5); d) hexagon (C_6) (**Figure 3**(**a**)–(**d**)). The polygons in amorphous solids are fundamentally different from all the molecules known in chemistry, of which about 20 million have been registered. The fact is that known molecules have strong covalent bonds. In contrast, atoms in polygons in amorphous solids are bound by unpaired electrons that form weak bonds. The thickness of the unpaired electron orbitals is approximately 40 picometers (green color).

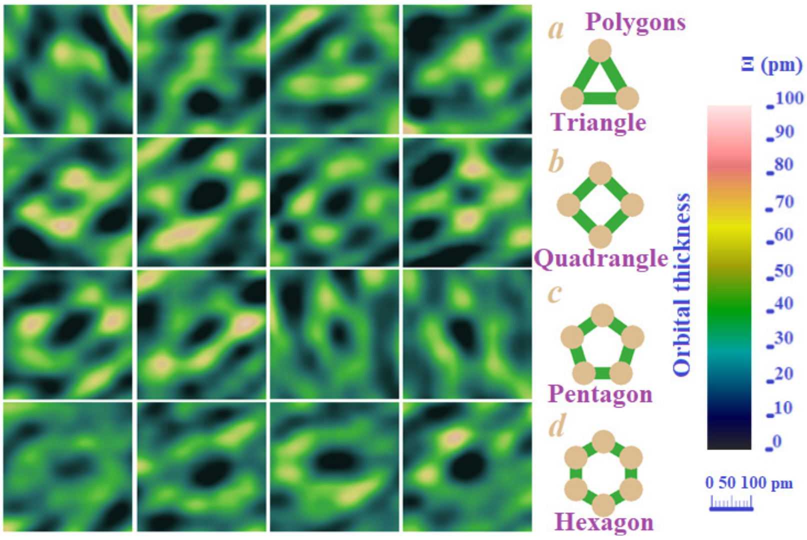

Figure 3. *Ξ*-Orbital Images of Polygons in Amorphous Carbon. General Formula Cn: (**a**) Triangle (C3); (**b**) Quadrangle (C4); (**c**) Pentagon (C5); (**d**) Hexagon (C6).

Each polygon represents a separate entity that does not interact with the others. For example, **Figure 3**(**c**) shows the rotational motion of a pentagon. That is, all four molecules are depicted at different angles. Several thousand polygons were analyzed. And a molecule with two atoms was never encountered. **Figure 3** convincingly shows that polygons in amorphous solids create a short-range order, but it does not extend further than 300 pm.

The results of the research show that the transition from a crystalline state to an amorphous state is not a simple reduction in the size of crystal grains. It occurs by changing chemical bonds, that is, through a chemical reaction. That is, crystalline translational symmetry is completely absent in amorphous solids. These are two different chemical substances. Accordingly, the amorphous solids are allotropes. In amorphous solids, atoms are bound by weak unpaired electrons, which are not replaced by other bonds when cooled, even close to absolute zero. Therefore, upon cooling, the viscosity decreases uniformly, which agrees with experimental data.

7. Allotropes of Carbon

Allotropes are different chemical compounds that consist of the same chemical elements. They have different geometric structures and different chemical and physical properties. The main characteristic that distinguishes one allotrope from another is the number of covalent bonds, i.e., hybridization. The largest number of allotropes is tetravalent carbon. It has two core electrons and four valence electrons. The most famous and widespread in nature are as follows.

7.1. Quadruple Hybridization

Diamond is the hardest transparent mineral in all regions of the spectrum (**Figure 4**). All four outer electrons are paired in the covalent bonds; the degree of hybridization is four.

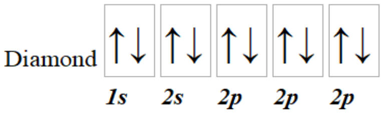

Figure 4. Molecular Orbitals of Carbon Atoms in Diamond: Two Inner Pink, Four Paired Yellow, and Unpaired Green are Absent.

7.2. Triple Hybridization

Graphite is a layered mineral that is opaque in all regions of the spectrum. The three outer electrons are paired covalent bonds, forming tetrahedral layers (**Figure 5**). The space between the layers is filled by unpaired valence electrons, one for each carbon atom. They form weak unpaired electron interactions between the layers.

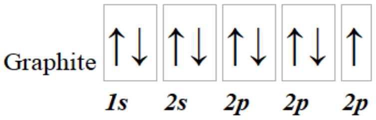

Figure 5. Molecular Orbitals of Carbon Atoms in Graphite: Two Internal Pink, Three Paired Yellow, and One Unpaired Green.

7.3. Double Hybridization

Carbyne, or a linear carbon as the third independent allotropic form of carbon, based on sp-hybridization of its atoms, can stably or quasi-stably exist only in the form of nano-sized structures (clusters) (**Figure 6**), so it should be considered not as an allotropic form of carbon in the usual stable sense, like graphite and diamond, but as a nanoallotropic form of carbon.

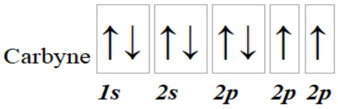

Figure 6. Molecular Orbitals of Carbon Atoms in Carbyne: Two Internal Pink, Two Paired Yellow, and Two Unpaired Green.

Additionally, materials based on carbyne can quite logically and reasonably be considered as cluster nanomaterials, which are a matrix of various kinds of carbon or other materials, including nano-sized clusters of doubly hybridized carbon.

7.4. Single Hybridization

The fourth allotropic form of carbon, when the atom has single hybridization, does not exist (**Figure 7**).

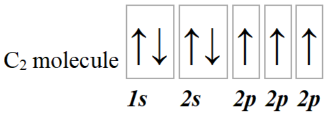

Figure 7. Molecular Orbitals of Carbon Atoms in a Diatomic Molecule: Two Inner Ones Are Pink, One Paired is Yellow, and Three Unpaired Are Green.

Carbon does not form a diatomic molecule, although diatomic molecules of hydrogen, oxygen, etc., are well known, where each atom has single hybridization.

7.5. No Hybridization

As shown by direct picoscopic studies presented in this article, amorphous carbon is a fifth allotropic form of carbon in which all four outer electrons are unpaired and, accordingly, there is no hybridization (**Figure 8**).

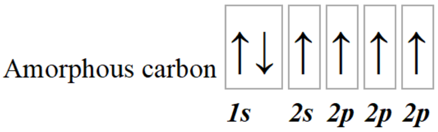

Figure 8. Molecular Orbitals of Carbon Atoms in Amorphous Carbon: Two Inner Ones Are Pink, Paired Yellow Ones Are Absent, and Four Unpaired Ones Are Green.

This is a new, previously unknown class of amorphous allotropes with no hybridization. Therefore, the presence of sp^2/sp^3 hybridization bands in the Raman spectrum of an amorphous sample indicates contamination of the sample with crystal impurities [9]. The presence of only unpaired electron interaction gives these compounds unique solid-liquid properties. When cooled even to zero, they do not form strong covalent bonds, do not hybridize, and, accordingly, do not have a crystallization point.

The diagrams show electron orbitals in different colors; the color corresponds to the thickness of the orbital according to formula (2) and the scale in **Figure 1**: ↑↓ inner paired, thickness 90 pm; ↑↓ outer paired, thickness 60 pm; ↑ outer unpaired, thickness 30 pm.

8. Discussion

Accurate measurements of the positions of atoms and the electron orbitals that connect them provide complete and reliable information for creating satisfactory theoretical models of amorphous materials. This information is sufficient to describe both the spatial structure and the energy structure. The lack of order and hybridization in amorphous solids, but the presence of polygons in amorphous solids and unpaired electron interactions, shows that the theory of amorphous solids must be fundamentally different from the theory of crystalline ones. The theory thus created will be exactly the impetus that is currently missing for the full use of amorphous materials in modern technologies.

9. Conclusions

The secret of the structure of amorphous materials has been revealed — in them: a) atoms are bound not by hybridization but by a dipole moment; b) the short-range order is determined not by the remains of the crystal lattice but by the presence of polygons. The basis of amorphous solids is the weak unpaired electron interaction, unlike crystals, which form a strong covalent bond. It is the unpaired electron that is the basis for creating a fundamental theory of amorphous solids and for mastering their limitless properties.

Picoscopic studies have shown that atoms in amorphous solids are bound by weak unpaired electrons, which are created by elongated Ξ-orbitals of unpaired electron interaction. That is, amorphous solids are new, previously unknown allotropes.

The polygons create a coordinated arrangement of nearest neighbors in amorphous solids. Their general formula is C_n: a) amorphous carbon (C_1); b) triangle (C_3); c) quadrangle (C_4); d) pentagon (C_5); e) hexagon (C_6).

It is polygons that are responsible for the universal spatial parameter of the order of ~300 pm, with which the structure of amorphous solids of various natures (semiconductor, dielectric, metallic) is associated. The unpaired electron interaction and polygons play a fundamental role in the nature of amorphous materials.

Direct visualization of real-life electron orbitals by picoscopy is a powerful tool in the study of amorphous solids. Picoscopy provides complete information about the position of each atom and the chemical bonds between them.

Author Contributions

Software, visualization, writing—original draft preparation, O.P.K.; conceptualization, investigation, writing—review and editing, A. D. R. All authors have read and agreed to the published version of the manuscript.

Funding

This work received no external funding.

Institutional Review Board Statement

Not applicable.

Data Availability Statement

The authors are willing to share research data via the website picoscopy.com or by email specified above.

Acknowledgments

The authors gratefully acknowledge the support from Center for Collective Use of Devices "TEM-SCAN", Institute of Materials Science named after I. M. Frantsevich, NAS of Ukraine, which provided facilities for this research.

Conflicts of Interest

The authors declare no conflict of interest.

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