

GLOBAL JOURNAL OF SCIENCE FRONTIER RESEARCH: A PHYSICS AND SPACE SCIENCE Volume 18 Issue 5 Version 1.0 Year 2018 Type: Double Blind Peer Reviewed International Research Journal Publisher: Global Journals Online ISSN: 2249-4626 & Print ISSN: 0975-5896

C & BN-Foundation for Atomic-Crystalline Orbitals

By Ordin S.V.

Ioffe Institute of the Russian Academy of Sciences

Abstract- The experimental data accumulated over a hundred years of modern physics, if brought together, can demonstrate "regularities" lying on the surface, which, sometimes, are not described by the "first principles." And this is normal, since the very first principles were formulated when, in the hands of the researchers, there was only a fragment that we now have in our database. So, as Planck demonstrated in his time, it is not surprising that the previously constructed basic models that abstractly describe the phenomenon from "zero" to "infinity", beyond the limits of their applicability, give singularities.

The quantum-mechanical model of a hydrogen-like atom constructed at the dawn of the last century described qualitatively the entire periodic table and made it possible to calculate atomic orbitals, in principle, for any quantum number. However, relativistic corrections were used to quantitatively match the allowed (model) energy levels. In addition, in order to describe chemical bonds in materials, the model orbitals were practically ejected and were replaced in the first approximation by the so-called hybridized ones.

These contradictions, in fact, were revealed in the complex analysis of C & BN, the results of which are presented in this paper. A general view of the hydrogen-like model of the atom showed that it gives a quantitative catastrophic divergence in the first order with an increase in the atomic number. Those. In fact, this model was linearly used, and 100% discrepancies were attempted to "correct" due to corrections in the order of smallness.

GJSFR-A Classification: FOR Code: 020399p



Strictly as per the compliance and regulations of:



© 2018. Ordin S.V. This is a research/review paper, distributed under the terms of the Creative Commons Attribution. Noncommercial 3.0 Unported License http://creativecommons.org/licenses/by-nc/3.0/), permitting all non commercial use, distribution, and reproduction in any medium, provided the original work is properly cited.

C & BN-Foundation for Atomic-Crystalline Orbitals

Ordin S.V.

Abstract- The experimental data accumulated over a hundred years of modern physics, if brought together, can demonstrate "regularities" lying on the surface, which, sometimes, are not described by the "first principles." And this is normal, since the very first principles were formulated when, in the hands of the researchers, there was only a fragment that we now have in our database. So, as Planck demonstrated in his time, it is not surprising that the previously constructed basic models that abstractly describe the phenomenon from "zero" to "infinity", beyond the limits of their applicability, give singularities.

The quantum-mechanical model of a hydrogen-like atom constructed at the dawn of the last century described qualitatively the entire periodic table and made it possible to calculate atomic orbitals, in principle, for any quantum number. However, relativistic corrections were used to quantitatively match the allowed (model) energy levels. In addition, in order to describe chemical bonds in materials, the model orbitals were practically ejected and were replaced in the first approximation by the so-called hybridized ones.

These contradictions, in fact, were revealed in the complex analysis of C & BN, the results of which are presented in this paper. A general view of the hydrogen-like model of the atom showed that it gives a quantitative catastrophic divergence in the first order with an increase in the atomic number. Those. In fact, this model was linearly used, and 100% discrepancies were attempted to "correct" due to corrections in the order of smallness.

This approach does not take logarithmic relativity into account ("Scientific misconceptions" Part III - <u>http://www.rusnor.org/pubs/articles/15503.htm</u>).

Correction of the external atomic orbitals of C & BN Pauling, taking into account the scale of the atomic number, resulted in the replacement of the hydrogen-like atom model by a model that takes into account the screening of the nucleus by internal electrons. And when describing many chemical elements within the framework of this quasi-nuclear model, the starting point is not a primitive hydrogen, but an elementary but not a primitive carbon atom.

So carbon, not only the basic element on the basis of which life on Earth arose, but also the basic element for describing many chemical elements. With this approach, the catastrophic divergence (singularity) is eliminated depending on the atomic number of the material properties.

I. INTRODUCTION

Well-known graphite and its white, dielectric analogue of boron nitride, first obtained from chlorides on laboratory work at the 3rd year of the Leningrad Institute of Technology by student Boris Sharupin, were rightly entered theorists into extremely anisotropic crystals from the existing on the Earth. But their high anisotropy was associated not with their most rigid connection of hexagons, but with the complete absence of chemical bonds in the crystal lattice between mono-atomic layers along the C axis. Although such so-called Van der Waals crystals without chemical bonds can exist only at helium temperatures, and C & BN do not fall apart and at 3000C, theorists "skidded".

The beginning of this "drift" can be related to the name of the classic, Linus Pauling, who invented sigma and pi-electrons [1].Although he personally found deep contradiction in his concept, and tried to introduce new, "curved" chemical bonds, the Van der Waals crystal model firmly entered the textbooks on solid-state physics under a modified name-two-dimensional crystals [2]. "Drifted" so far that the difference between real C & BN crystals from two-dimensional ones tried to describe, in the form of quasi-two-dimensionality, small corrections to the two-dimensionality. And the majority, like the same Dresselhaus, where we should "remember" about the two-dimensionality, and where it should be "forgotten". By the same principle, the nonexistent "graphene" even "earned" the Nobel Prize.

Doubts in some basic physical models initially arose in my analysis of the anomalies of crystal optics of incommensurate crystals. But the optical anomalies observed on them I considered quite natural for a qualitatively new four-dimensional object [3].

However, I decided to test the crystal-optical models of plasma and lattice oscillators on the asymptotic behavior of the anisotropy of classical crystals, on an "ideal" anisotropic conductor -graphite, and on "ideal" anisotropic dielectric-boron nitride.

But the first experiments on C & BN samples (and on the grown by B.N. Sharupin [4], and on American), showed that:

- 1. and the samples are far from ideal crystals,
- 2. and the fact that their properties are not described by ideal models in any way (as indicated by the authors of the first papers [5]).

And now, after 7 years of our joint work, BN. Sharutin grew "ideal" C & BN crystals, and I experimentally examined them, and showed that:

3. properties of C & BN and can not be described by two-dimensional models, since they do not take into account chemical bonds between atomic planes.

Author: e-mail: stas_ordin@mail.ru

And then me, a young employee, a venerable scholar BN. Sharupin invited me to a conference on the conference he was holding at the First Atomic Station of the USSR. He invited me to a report refuting what was written in the books, including what was written in his book, with a report refuting the van der Waals interaction between monoatomic layers in C & BN.

Perestroika, one can say bluntly, killed Boris Nikolaevich. And the results we have obtained, I was able to publish in a physical journal, only after including it in co-authors posthumously [6].

But there was a gap between purely physical, inconsistent with the usual notions, the conclusions of our publication and a huge layer of purely technological research by Sharupin's staff, without which it would be impossible to obtain perfect crystals and, as it turned out, understand and accept our conclusions.

His hole was reflected in the books published after our work. Even in the handbook published in Schringer by the employee of our Institute, the conclusions of our publication on the basis of a huge number of little-known works by the best technologists of the world were not reflected (when Japanese Americans learned to grow perfect crystals 5 microns thick, Boris Nikolayevich gave me more palm- on which I measured all the crystal optics, and not just the normal planes, which is reflected in our publication). Partially this hole I tried to fill with physical research, spent some time with the former (in GIPH) officers B.N. Sharupina. But the great purity of the results obtained was published only in the works of Russian conferences [7 -12] and are not known in the world so far.

Now, when the world began to be interested in my previous publications, I was asked to send their originals. But in post-perestroika time not all reports of Russian conferences were published. To some extent, this prompted me to write a book in which not only the final conclusions for ideal anisotropic crystals are shown, but also shows a purely experimental basis for the observed regularity-the dependence of the physical properties of the pyrocrystals on the ordering degree of both their crystal lattice and the complex ordering hierarchy crystallites.

But when analyzing the structure and properties of C & BN [13, 14, 15, 16, 17], a catastrophic discrepancy was revealed in the most general physical laws. The dependence of the upper filled level on the atomic number within the base model of the hydrogenlike atom is qualitatively different from the experimental data on the first ionization potential, and the atomic orbitals calculated to arbitrarily large principal quantum numbers are not the first approximation even for the elementary carbon atom (require 100%). Soitturnedout that

1. that an elementary, but at the same time, nonprimitive carbon atom, and not an ideal model based on the hydrogen atom, is a "brick" for atomic physics and the description of chemical bonds.

So, the "brick" of organic life carbon is the real "brick" of atomic physics, and graphenology takes away from reality even the physics of carbon itself.

The research of C & BN was also of a purely applied nature. In particular, the C + BN composites tested not only the correctness of the use of optical models for interpreting the properties of incommensurate superstructure crystals, but also the analysis of the effect of potential barriers on efficiency [18]. And thermoelectric although a conductive C + BN was obtained, and its Seebeck coefficient exceeded the thermoelectric power of pure graphite by a factor of tens, but it reached only 500 μ V / C and did not find any practical application.

However, these experiments put the finishing point in the analysis of barriers, showing the need for artificial asymmetry of the barrier on a nano scale. So C & BN to the formation of semiconductor structures with local thermo-emf [19-24]. Now the circle is closed - the analysis on the basis of C & BN allowed levels (zones) of electron energy has made it possible to come closer to an understanding of "What materials and how to make artificial semiconductor structures with high energy conversion efficiency.

II. BASIC SIMILARITY AND DIFFERENCE Between c & bn.

C & BN are the most elementary similar in basic parameters compounds for a whole class of actively used elementary semiconductors Si and Ge and similar and semiconductor-analogues A3B5: Si & AIP (N, As), Ge & GaAs (P, Sb), Sn & In Sb ((As, Bi). namely, the elementary nature of C & BN at the atomic level makes it possible to estimate with good accuracy also their crystal properties at the lowest, atomic level, which allows them to be used as a base point of departure for the whole class.

a) Similarities of C & BN, which give the overall picture

Although the hydrogen-like model of atoms used for the qualitative explanation of atomic-molecular bonds of any chemical elements of the Mendeleyev table gives significant quantitative discrepancies with experiment already in the first period, it nevertheless describes fairly well the first two periods. Moreover, as will be shown below, the quantitative discrepancies observed in these periods with experiment indicate the need for modification of the elementary model, the possibility of its modification, and the possibility of using (at least in principle) at least the DEFINITIONS s and p orbitals of the hydrogen-like model, and! - the similarity of electronic orbits C & BN. And although the number of external electrons in boron and nitrogen is different, but their external orbitals (allowed in the atoms of the electron state) are similar and, therefore, external electrons are distributed between the boron and nitrogen atoms approximately in carbon. At the same time, both materials have 4 valence electrons per atom. As a consequence, the crystalline structures of all phases of BN are in many respects similar to the corresponding structures of C (similar to the rest of A3B5, the similarity to the structures of the corresponding elements of the fourth group is observed). And, as a result, the phase diagrams of graphite and boron nitride are similar (Fig. 1).



Fig. 1: Similar phase diagrams of carbon (the boundaries of the phases are marked in green) and boron nitride (the boundaries of the phases are marked in red). Conditionally, the boundaries between two cubic phases of carbon and a metallic "diamond" are shown.

In the low-pressure region, both materials exist layered modifications: hexagonal in two and rhombohedral, in the spirit phases, which are different, as will be shown in the analysis of lattice vibrations, not by the rigidity of interatomic bonds, but by their ordering. In the high-pressure region, two cubic modifications are observed: brittle, diamond-like, with bond stiffness about 30% lower than in hexagons, and the γ phase is elastic-viscous, diamond-like, but with interatomic bonds close to the interlayer in layered phases. At very high pressures, the existence of a denser metal phase than diamond is assumed, which corresponds to the realization of a diamond structure with four internal hexagonal bonds.

Although the boundary between layered and cubic modifications strongly depends on time and catalysts, the fundamental similarity of phase diagrams further confirms the similarity in them of the transformation of atomic orbitals into crystalline ones and the similarity of the transformation of crystalline orbitals during phase transitions. Some displacement of the boundary layer / cube transition for boron nitride in the low-pressure region can be attributed to an additional, naturally, contraction due to the additional ionic contribution to the potential energy of the crystal. A shift in the boron nitride of the solid-phase transition to lower temperatures is associated with an additional contribution to the kinetic energy of the crystal due to ion oscillations (optical branches).

The rhombohedral phase of graphite was not observed in nature at all, which led earlier to draw the wrong conclusion that in boron nitride and in graphite it is under normal conditions a metastable phase (like a diamond). While experiments on the annealing of perfect rhombohedral boron nitride crystals directly, on the transformation of lattice oscillators, have shown a phase transition at a temperature of about 1250C to a hexagonal state. So, and hexagonal C & BN hexocarbon crystals, as well as natural hexagonal graphite, under normal conditions, are just in a metastable quenched state, but in a stable as a diamond. And just like a diamond, the hexagonal phase can not be transformed into rhombohedral phase at low temperatures because of large interatomic forces in the plane of hexagons and 2018

because of the very low rate of the solid phase transition [16, 17].

A rigorous three-dimensional one, taking into account interplanar ion-covalent bonds, the ordering of the crystal lattices of C & BN is possible only in the rhombohedral phase (with a translation period along the C axis equal to the tripled interplanar distance). And, as is clearly seen in the construction of the crystal lattice of boron nitride, the doubled interplanar spacing observed in the hexagonal phase does not correspond to the translational invariance of the interplane bonds. Thus, the hexagonal phase, in principle, corresponds to a random (with defects) distribution of interplane bonds, and the rhombohedral / hexagonal phase transition is an order-disorder transition in their distributions (between layers). This chaos leads to a high slip of the layers (potential minimum blurred-wide), and the formation of solitons in the distribution of interlayer bonds, contributes to the formation of small-crystalline

polycrystals, and as a result, to slip and cleave only crystallites (flakes).

Cubic modifications of C & BN also exist and were studied in two phases. In the form of a so-called gamma phase, obtained by the hydrostatic compression method or by explosion from a hexagonal or rhombohedral phase of a denser, diamond-like package, and in the form of a hydrostatic compression from the so-called isotropic C & BN pyrocrystals of a more loose package. But as will be shown in the analysis of lattice reflection, the so-called amorphous C & BN obtained is also a cubic C & BN, differing not only in the space symmetry group, but in the rigidity of the interatomic bonds.

Similarity is manifested in the growth of C & BN, and the technology of their cultivation [4], and in the microstructure arising in the microcrystals.

The least ordered and the least dense phase is the so-called pipe-stratum phase (Fig. 2).



Fig. 2: Electron microphotographs of the pyrolytic crystals of the C-BN pipeline stratum: a and b are the plane parallel to the growth axis C (preferential orientation of crystallographic axes of microcrystallites), c is the plane perpendicular to the growth axis (the edge of the figure is approximately 1 mm).

The micrographs of the pipe-stratified phase shown in Fig. 3.1 have an almost equivalent character, both for graphite and for boron nitride. They demonstrate what follows from the whole complex of studies, and from the natural nano-state of C & BN - the appearance of embryos in the form of fulerenes. As shown in [1], the natural state of embryos from atoms: three (rigid, "straight") orbitals are closed to neighboring atoms in a collapsed plane, and the fourth orbital (softer, but not a "curve" according to Powling), closing to a similarly torn interlayer orbital of one of the neighboring atoms of the same layer. This leads to the specification of the curvature of the surface of the mono atomic layer. As shown in Fig. 3, some amount of fullerene-like defects is also observed in the most perfect samples of the rhombohedral phase.



Fig. 3: A microphotograph of the growth defect, whose small concentration is also observed in perfect rhombohedral C & BN rhombo-crystals.

Under conditions of a lot of germinal growth of a hexagonal-linked cryocrystal, a weakly ordered least dense, the least anisotropic (as will be shown below), a brittle, coarse, low-density, pipe-stratified phase appears in the layer. As can be seen from Fig. 2, these cryocrystals are textured polycrystals consisting of interlaid spacing packets with a large spread and the mean orientation of the C-axis of the packet, and the orientation of the C-axis of the stack. At high precipitation temperatures, hexagonal pyrocrystals with a low concentration of growth cents with a much higher density and with a strict orientation of the C-axis of the packets, but precisely packets of fine and well-ordered crystallites, can also be formed (Fig. 4).



Fig. 4: Electron micrographs of hexagonal C and BN hexagonal pyrocrystals: a and b - a plane parallel to the growth axis C - the preferential orientation of the axes of microcrystallites C, c is the growth surface (perpendicular to the C axis).

In this case, as can be seen from Table 1 and Fig. 5, the degree of ordering of the crystallites (including the transitions between the phases: trubostrata - hexagonal-rhombohedral - uniquely correlates with the degree of disorder of the interatomic distance in hexagons, which we will use later for

quantitative characteristics and microstructure and physical properties of pyrocrystals.

Type pyrocryst- als	Rh	Ge	High-density pyrocrystals			Low-density pyrocrystals				lsotropic pyrocrystals		
N°	0	1	2	3	4	5	5'	6	7	7'	8'	8
d,Å	3,34	3,36	3,37	3,38	3,41	3,44	3,44	3,44	3,44	3,44	3,44	3,44
δd,Å	0	0,005	0,018	0,022	0,13	0,2	0,22	0,23	0626	0,16	0,18	0,21
a, Å	2,46	2,46	2,46	2,46	2,46	2,46	2,46	2,46	2,46	2,46	2,46	2,46
δa, Å	0	0,001	0,003	0,006	0,01	0,011	0,012	0,015	0,019	0,010	0,011	0,019
L _C ,A	2000	1000	275	260	111	80	84	30	20	154	110	90
La,Å	8	>104	320	359	70	45	42	32	25	58	50	47
ρ, g / cm ³	2,26	2,25	2,24	2,23	1,86	1,86	1,76	1,6	1,34	2,08	1,9	1,82
ρ*, g / cm3	2,26	2,247	2,24	2,233	2,214	2,194	2,194	2,194	2,194	2,194	2,194	2,194
Δγ,°	0	0	20	25	30	45	50	55	60	90	90	90

Table 1

As can be seen from Table 1, the x-ray density ρ^{\star} of weakly ordered samples is above the pycnometric density ρ , which is due to the presence of voids in these samples. In this case, the crystal-like,

phase transformations of the crystal lattice of pyrocrystals from Table 1 were obtained by comparing the microstructure with X-ray spectra (Fig. 5).



Fig. 5: Correlation of a complex hierarchy of ordering of crystallites with the ordering and structure of the crystal lattice of C & BN based on the results of X-ray structural measurements and electronic photographs of the plane parallel to the growth axis of a series of samples of different phases of C & BN with different degrees of ordering of the crystal lattice and microcrystals: a is a highly ordered rhombohedral, b mixture of layers of rhombohedral and hexagonal, c - highly textured hexagonal, d - low-order hexagonal and e - the so-called pipe-stratum phase a.

© 2018 Global Journals

As seen from Fig. 5, the most ordered crystal lattice, and the maximum size of highly ordered crystallites, are the C & BN pyrocrystals of the rhombohedral phase. At the same time, the change in the interatomic distance in hexagons when the samples are disordered is practically determined by its own

blurring δa (Tab.1). This is quite natural, since hexagonal links are the toughest in C & BN. Therefore, a clear correlation is also observed between the interplanar distances in the crystal lattice (Fig. 6a), and the crystallite size of the C & BN pyrocrystals.



In the dependences of the additional (on the binding energy) parameter of the C & BN crystal lattice and the sizes of the crystallites on the parameter δa , which is characteristic of the ordering of bonds in hexagons, the parameter δa is clearly seen in certain regularities. The relatively sharp growth of interplanar parameters at the initial section is accompanied by a transition from a three-dimensionally ordered rhombohedral phase into a two-dimensionally ordered one. Hexagonal and a sharp reduction in the size of crystallites with a decrease in their geometric anisotropy.

Further, there is a slow increase in the interplanar spacing d (which correlates with a slow decrease in the LC crystallite size along the C axis), but a faster increase in the blurring of the interplanar spacing δd (which correlates with a faster decrease in crystallite sizes along the La hexagon layers, leading to the disappearance of their geometric anisotropy, and then to its inversion).

In the third segment, the growth of the interplanar distance is again accelerated, although being much smaller than the blur, and it itself is already determined by the blur, and further diminution of both sizes of crystallites is also determined by this blurring. This blurring of the interplanar distance also determines the further decrease in the crystallites in the fourth section. But within the crystallites, a further increase in the interplanar distance is impossible, as shown by the d (δ a) observed in the fourth section. And this shelf is an additional confirmation of the existence of interplanar connections in C & BN. It gives the maximum length of the "interplanar" orbitals observed (as will be shown below) in the cubic gamma phase.

Isotropic pyrocrystals - polycrystals obtained from technology with a high concentration of nuclei from randomly oriented small hexagonal crystals (sometimes called the "amorphous" phase), as seen in Fig. 6, also fit into the described regularities with some quantitative correction.

b) Differences between C & BN, which complement the overall picture

The band structure of layered carbon modifications and boron nitride is fundamentally different because of the presence of a dipole in the latter. As a consequence of the large difference in the concentration of free carriers, their electrical conductivity and other kinetic parameters are radically different. But the electronic contribution to the binding energy of atoms in the lattice and in graphite is much less than the binding energy between the mono-atomic lavers. Therefore, the kinetic properties of graphite characterize the given crystal lattice in general. On the other hand, a slight difference in the charge and mass of the boron and nitrogen atoms, which have become in many respects equivalent in the crystal lattice of boron nitride, are reliable markers, which, as will be shown, make it possible to exclude irregularities that violate the

translational invariance of the arrangement of monoatomic layers. In addition, the presence of a dipole in the boron nitride lattice makes it possible to analyze quantitatively the strength of interatomic bonds also in general, because The energy of the dipole interaction does not substantially distort the crystal lattice.

Therefore, the difference in the properties of C & BN not only does not interfere with the analysis of their physical properties, but even helps. And the kinetic properties of the ideal conductor (which does not have dipole scattering) of graphite, and the optical properties of the ideal (practically free of the masking contribution of free carriers) of the boron nitride dielectric and are in good agreement with the "similarities" listed above, and even supplement / explain them. The results of the experiments presented in this section will be used rather to demonstrate the manifestation of the "similarities" noted above (and their complements). Although, along the way, taking into account and clarifying the identified "similarities," some adjustment of the commonly used working models will be carried out.

i. Dependence of the kinetic parameters of C & BN on the degree of ordering

Studies of graphite, both natural crystals and pyrographite, have been devoted to many works [25-43]. And not by chance, since it is a unique material.

The electrical conductivity over the layers of graphite hexagons is in some ways unique, especially its anisotropy, reaching a million. But the use of the Van der Waals assumptions [44], rather, made it difficult to understand the true nature of it, than it helped. So the highest anisotropy of the electrical conductivity was attributed not to the peculiar motion of the current carriers along the hexagons (as was pointed out for a long time by the giant oscillations of de Haas-van Alphen oscillations in graphite), but with the alleged total absence of electron overflow from one mono layer another. Then, as shown in Fig. 7, the dependence of the electrical conductivity on the basic ordering parameter of the C & BN crystal lattice directly gives a different explanation.



Fig. 7: Dependence of the electrical conductivity along σ_a and across σ_c of the mono-atomic layers of graphite on the hexagon ordering parameter δa .

From a comparison of Figures 7 and 6, it is clearly seen that a sharp drop in the initial (first) section of σ_a and σ_c occurs during a transition from a threedimensionally ordered one, and as a consequence, having a considerable conductivity across the mono atomic layers, the rhombohedral phase into a twodimensional ordered hexagonal phase. However, a catastrophic decrease in macroscopic σ_{c} during the transition to a highly ordered and strictly textured hexagonal phase occurs not only due to the termination of the flow of electrons between mono atomic layers (the concentration of interlayer bonds in the hexagonal phase is not much smaller than in the rhombohedral phase, they are simply disordered), but and because of the concomitant decrease in the crystallite thickness along the C axis by an order of magnitude (for the rhombohedral phase of macroscopic packets with thicknesses of thousands of angstroms).

Scattering of electrons at the boundaries of crystallites in the hexagonal phase gives a significant contribution to the macroscopic resistance of hexagonal pyro graphite along the C axis, and the weak, almost van der Waals bond between the crystallites, determines the high sliding of the "layers" of graphite against each other. She also ensured the possibility of obtaining a Nobel Prize with the help of a sticky tape "inventors" of graphene.

A fundamentally new for understanding / explaining "similarity" gives a subsequent sharp rise in the electrical conductivity σ_c at the boundary of the first and second sections. Since no growth of crystallite thickness is observed at all, and no sharp disruption is

observed, a sharp increase in the electrical conductivity of the pyrocrystal along C indicates that a critical disruption of the ordering of hexagons in the grid leads to interlacing of hexagonal nets.

The course of the dependence of the electrical conductivity on the further increase in the disordering of hexagons is in good agreement with the regularities shown in Fig. 6 and have not revealed anything radically new. And the main interest was the properties of highly ordered pyrocrystals of the hexagonal and rhombohedral phase. Therefore, without dwelling on the model description, just to demonstrate the abovedescribed regularities, we will give the polarization spectra of the plasma reflection of pyrocrystals of different degrees of ordering (Fig. 8, where the sample numbers correspond to Table 1).



Fig. 8: Conjugated with reflection of local plasma oscillations, the polarization spectra of plasma reflection on free carriers for pyrographs with different degrees of ordering: 0 - rhombohedral crystal, 1 - highly ordered hexagonal phase, 2 and 3 - hexagonal phase with increasing degree of disordering of hexagons.

As can be seen from the comparison of spectra 0 and 1 in Fig. 8, the transition from the rhombohedral phase to the hexagonal leads, primarily to a sharp decrease in the conductivity along the C axis. Moreover, it is seen from the high-frequency part of the reflection spectra that there is a mixing of localized plasma oscillations and, respectively, the transformation of the electronic band structure. And when passing from spectrum 1 to spectrum 2 with E || C, an increase in plasma reflection is observed, analogous to an increase in the electrical conductivity σ_{C} at the boundary of the first and second sections of Fig.7. That is, the dependence of the reflection on free carriers on the degree of ordering is similar to the analogous dependence of the anisotropy of the electrical conductivity on a direct current.

Also briefly, without going into the description of experiments at different temperatures, we demonstrate the effect of disordering hexagons on the thermoelectric power of pyrographs along and across the C axis at one room temperature (Fig. 9).



Fig. 9: Dependence of the thermoelectric power along a_c and across a_a axis C at room temperature on the degree of ordering of hexaons δa .

As can be seen from Fig. 9, up to room temperature, the thermo power in perfect rhombohedral pyrographite is practically zero for both crystallographic directions. Those, despite the giant anisotropy of the electrical conductivity, and along the C axis, and across it the ideal graphite behaves like a good semimetal in which the contributions to the conductivity are weak, that is, the active losses due to interband / phonon scattering are small in both directions.

Moreover, for a_a these contributions are small up to the critical value of the disordering of hexagons corresponding to the boundary of the fourth section in Fig.6. However, for the direction along the C axis, the active scattering processes that determine the diffuse Seebeck coefficient are sharply manifested in a_c starting from the minimal degrees of disordering of the hexagons. This is quite natural, because In the first place, weaker interplane bonds / orbitals are destroyed.

The anisotropy of local plasma oscillations (curves 0 for E parallel and perpendicular to the C axis) observed at the high-frequency edge of the reflection spectra (Fig. 8) of rhombohedral pyro graphite sharply decreases upon transition to the highly ordered hexagonal phase, while the low-frequency reflection anisotropy on free carriers, in full agreement with anisotropy of DC conductivity, maximum.

From the analysis of the influence of the degree of ordering of hexagons on the kinetic and optical parameters, one can make an unambiguous conclusion that the ideal rhombohedral graphite has not an abstract two-dimensional conductivity and a mythical dielectric nonconductivity along the C axis, but an ordinary semiconductor one. And, from the corresponding reflection spectrum "0" at E // C, the refractive index of the order of 3, follows the width of the forbidden band $E_g \sim 1.6 \text{ eV}$. I'm not sure that anyone measured the width of the forbidden zone of the van der Waals crystal, but I think it is no less than 10 eV.

The results obtained make it possible to construct a band model of graphite qualitatively describing the change in its properties with a change in its degree of disordering and eliminating the contradictions inherent in the Slonchevsky-Weiss band model for ideal graphite [26]. In addition, the proposed model has fewer in dependent parameters, so all the described experimental results can be explained without using additional, heavy b ands for electrons and holes [42].

The internal contradiction of the CB model is due to the mutually exclusive assumptions: on the one hand, it is assumed that the lattice of an ideal graphite corresponds to a strictly two-dimensional material, that is, with an infinite effective carrier mass in the C direction; on the other hand, finite effective electron masses and holes. The three-dimensional correlation observed in x-rays in the crystal lattice of highly ordered pyrographs is in complete agreement with the physical properties of these materials described above. Therefore, the widely used purely two-dimensional band conduction model in graphite (Fig. 10a) can not be accepted even for the coarsest approximation.

The band structure of graphite, in the first approximation, should be described by the model depicted in Fig. 10b.



Fig. 10: Model of a two-dimensional zone (on the left) and a zone of 3-dimensionally ordered graphite (right).

The principal point of the proposed band model is that the semimetallic overlap is indirect, since the maximum and minimum of the zones are spaced in the k space along k_c The placement of electrons and holes in energy-overlapping bands, which are not overlapping in the pulse, explains their small mutual scattering (at not very low temperatures, when the phonon momentum is less than the displacement due to the momentum of the extrema-the total absence of scattering). On the other hand, the motion of the current carriers along the C axis has an additional reactance connected with the need to overcome a potential barrier equal to the width of the forbidden gap shown in Fig. 10.

Thus, the limiting anisotropy of an ideal graphite is determined by the fact that it is semimetal along the planes and the semiconductor is perpendicular to it. But the estimate of the width of the forbidden band obtained earlier on the basis of an empirical relation for isotropic semiconductors gives an obviously overestimated value. Therefore, direct measurements of the energy gap were made by passing thin dispersed graphite films deposited on an IR transparent substrate (Fig. 11)



Fig. 11: Absorption spectrum of a film of finely dispersed pyrographite.

Dispersing graphite eliminated through conductivity, masking narrow slit effects.

The obtained absorption spectra of pyrographs are well described by the additive contributions of two processes:

indirect permissible transitions: $\alpha \sim (E - (\Delta E_1 + E_{ph}))^2$, with the characteristic frequency $(\Delta E_1 + E_{ph})/h = -640$ cm⁻¹, where E_{ph} is the phonon frequency and by direct allowed transitions: $\alpha \sim (E - \Delta E_2)^{1/2}$, with $E_{ph} / h = +$ 1000 cm⁻¹.

Taking into account that the maximum phonon frequency for graphite is about 1400 cm-1, the obtained values of the edges of the inter band transitions correspond to a band structure with a direct slit near the Fermi level of about 0.125 eV and an indirect overlap of 0.25 eV. From the above analysis it follows that with a decrease in the degree of disorder in pyrographs, the forward energy gap decreases, and the overlap of the zones increases.

ii. Dependence of C & BN optical parameters on the degree of ordering

Pyrocrystals of boron nitride, as well as graphite, are a unique technological and technical material, inferior to pyrography only in heat resistance, but superior in diffusion of impurities (diffusion gate) and in radio transparency. Therefore, since the creation of boron nitride BN Sharupin, he was also actively investigated [11-17, 45-50].

The optical properties of graphite have already been used in analysis. But many optics and optically useful optical effects in highly conductive graphite are strongly shielded by current carriers. Therefore, they are either practically inaccessible for measurements, or require special indirect methods: measuring - the type of disturbed total internal reflection and technological - the type of graphite dispersion described above, in order to suppress through conductivity at the wavelength of the radiation used for the diagnosis.

Both the first and second numerous, and not only the above methods, were used to analyze C & BN. But they were used only for qualitative, testing analysis. As with the correct modeling of physical processes, it is necessary to build on the model describing the effect in the first approximation, and not in the form of the tenth correction, and with the right experiment, one must build on a reliably established direct effect, and not indirect ones.

In this respect, the Raman scattering, which has become fashionable and in many respects superseding classical spectroscopy, is by definition an indirect effect, i.e. interpretation of the results of these measurements is incorrect without reference to the base effect. In addition, the indirect effect of the effect also strongly influences the experimental conditions: the radiation flux used is many orders of magnitude greater than the fluxes of nondestructive IR spectral diagnostics, and the recorded signals, which are attenuated by 7 orders of magnitude, are also orders of magnitude lower than in classical spectroscopy. The same can be said about the use (mainly because it has nowhere to go for the colliders) of synchrotron radiation. But it is better to talk not about what is useless or unreliable, but about what is useful. Classical spectroscopy, in principle, allows recording directly, in reflection, many effects even in highly conductive samples. But for this it is necessary to take into account the general phenomenon - logarithmic relativity and to increase the accuracy of measurements. And this was also repeatedly tested and used. The results presented below were interpreted taking into account the logarithmic dependence of the responses, and were measured not with a standard "optical" accuracy of 2-3%, but with an accuracy of the order of one thousandth percent. To increase the sensitivity of the optical technique, the optical zero was improved and a computer technique for noise analysis was used.

But, in addition to the measuring technique, it is also necessary to have an "instrument" - an effect that gives directly and unambiguously information, in our case, a crystal lattice. And in boron nitride, this "tool" is a residual "memory" of the fact that the boron and nitrogen atoms are different, the dipole in the crystal lattice allowing both the recording and stiffness of the interatomic bonds and the degree of ionicity of the dipole to be recorded both directly and in reflection [51]. As was shown above, the contribution of this dipole in boron nitride (and its difference from the contribution of a small concentration of free carriers in graphite) can be neglected to a first approximation. And the change in the parameters of the same type of crystal lattices during the transition from boron nitride to graphite is less than their change in phase transitions and disorder, and the above C & BN characteristics, starting with their phase diagrams, are similar and differ onlv quantitatively. Therefore, the results of the dipole analysis of the crystal structure of boron nitride are also applicable in the first approximation to the crystal structure.

The polarization spectra of the lattice reflection of a perfect rhombohedral boron nitride picr crystal are shown in Fig.12.



Fig.12: Lattice reflection spectra of perfect (with a low concentration of defects and penetrating at several millimeters thick) crystals of boron nitride: rhombohedral phase (a and c) and diamond-like cubic phase (b).

The reflection spectra of rhombohedral boron nitride shown in Fig. 12 demonstrate practically ideal, weakly damped lattice oscillators that exist in the lattice in both the hexagon plane (Fig. 12a) and between the mono-atomic layers (Fig. 12c). In this case, the frequency of transverse vibrations (the low-frequency edge of the lattice peak) characterizing the rigidity of atomic bonds is approximately 1.8 times lower for interlayer bonds than for bonds in hexagons. In addition, the width of these oscillators, and strictly - the difference in the squared frequencies of the high-frequency edge of the grating oscillator (longitudinal vibration) and the said low-frequency gives the ratio of the concentration of dipoles in the shown orthogonal directions 1: 3. This ratio strictly corresponds to the ratio of the number of orbitals between the layers and in the layer and shows that all 4 external electrons are involved in the lattice on ion-covalent bonds. And the limiting anisotropy (with respect to the lattice stiffness) is not a theoretical twodimensional infinity, but 1: 7.2

Fig. 12b shows a lattice oscillator of a cubic, diamond-like, equivalent in hardness, but more durable and wear-resistant boron nitride obtained by the rhombohedral explosion method. Its grating oscillator is also sufficiently weakly damped. And although the damping of this oscillator appears somewhat more than in the rhombohedral phase, and directly from the graph, the model processing of the spectrum also gives the stiffness of the interatomic bonds intermediate between the interlayer and interlayer bonds, and the width of the peak gives the concentration of dipoles 4 per atom, i.e. the total number of orbitals per atom.

2018

Thus, in the phase transition from the rhombohedral phase to this cubic phase, the orbitals of the hexagons are somewhat stretched, and the interplanar orbitals somewhat contract and move to the mean equivalent position. The transformation of the lattice described in boron nitride is even more natural and rigorous for graphite, but the assumption that there is no chemical bond between the monoatomic layers in graphite, as will be shown below, is unnatural!

Naturally, before the results shown in Fig. spectra of reflection and before the presented

conclusions were made, the whole series of samples of boron nitride with different degrees of ordering of the crystal lattice was obtained and investigated. For a logical description it is necessary to go in the reverse order and in the following figure 13 the spectra of the reflection of a pyrocrystal with a minimum degree of disorder are presented - a strictly textured hexagonal boron nitride boron crystal.



Fig. 13: Polarization spectra of lattice reflection of strictly textured hexagonal boron nitride.

Just as in a rhombohedral crystal, the reflections of three normal modes were studied to control the dependence of the optical properties of the crystal on the orientation of the wave vector relative to the crystallographic axes. Spatial dispersion, which is manifested as a first approximation in long-period structures, is not revealed here, and the crystal-optical effects due to the smallness of the disorientation of the crystallites and their size are much smaller than the lengths of the investigated waves, also were insignificant (in contrast to weakly ordered pyrocrystals, where they are large).

So, the mixing of normal oscillators (the transformation of the shape of the oscillator due to the

"creeping" for a given polarization of the oscillator), which is observed in the reflection spectra of the hexagonal phase, strictly corresponds to the mixing of orthogonal oscillations in the crystal lattice itself due to the previously described disruption of the ordering of the interlayer bonds (and the concomitant entanglement of neighboring hexagonal meshes on solitons - boundaries of crystallites). The corresponding "overflow" of normal vibrations in the hexagonal phase is also clearly seen in the absorption spectra of the plates perpendicular to the C axis shown in Fig.14



Fig. 14: IR absorption spectra of rhombohedral and hexagonal boron nitride (against the backdrop of reflection of a rhombohedral crystal).

The IR absorption spectra shown in Fig. 14 clearly show that in addition to the "allowed" (in the orientation of the wave vector and polarization) high-frequency high-power absorption band in the region of 1372 cm-1 in the region of transverse "forbidden" oscillations along the C axis at 763 cm-1 in the hexagonal phase, a sufficiently powerful absorption band characterizing the energy flow is also observed. In the rhombohedral phase, there is also a "strange" band in this region, but this, as shown by a special polarization analysis, the transmission-scattering band, whose shape depends on the aperture, and whose nature is the parametric interaction of modes, present in principle, in any, even ideal anisotropic crystal.

The used rhombohedral and cubic samples had insignificant scattering on the defects, but so insignificant even in the ultraviolet, that it did not interfere with the measurement of the absorption spectrum (Fig. 15 from above) and reliably determine the width of the forbidden band (Fig. 15 from below).

2018

© 2018 Global Journals



Fig.15: Absorption spectra in the region of interband transitions of various modifications of boron nitride.

Whereas the haze of a large-grained textured hexagonal sample, as shown in the upper Fig. 15, it was not possible to determine its width optically.

The dullness obtained from an isotropic sample at relatively low pressures of the cubic gamma phase was also high, but in the IR region, due to the smallness of the crystals, its mirror grating reflection was reliably recorded (Fig. 16).



Fig. 16: Comparison of lattice oscillators of gamma-phase with intralayer in hexagons, with diamond-like and interlayer oscillators.

The spectrum of lattice reflection of the boron nitride gamma phase directly demonstrates that in this cubic phase there is an interatomic orbitals akin to interplanar in the rhombohedral phase.

III. Analysis Of Resolvedenergy Level Of Electron

For chemical bonds, first of all, the upper electron-filled atomic level (which corresponds to the first ionization potential of the atom and the work function of the solid body formed from these atoms) is important, and the empty level closest to the filled level (which corresponds to the electron affinity).

On the example of the "elementary" C & BN, the relationship of the macroscopic properties of a substance with properties at this "elementary" atomic level can be continued, at the same time, and correcting it, rather than confining itself to its statement in the introduction. And on the atomic level, this chain has necessarily continued with the correction of the basic model of the crystal bonds of the "elementary" C & BN [6]. Elementary C & BN can only be said to be He and Li, but only the simplest s-orbital is filled with them. And for most materials used, the electronic structure is richer and it needs to be represented in the first approximation.

Such a correct approximation, in fact, is the model of the electronic structure of C & BN, and not the model of the hydrogen atom. While most calculations of atomic orbitals of complex atoms (electron density distribution) are conducted in the form of numerous corrections to the model of the hydrogen atom. Here is a refinement of the C & BN crystal model based on electronic orbitals and led to the need to comb the model of the atom, which, in principle, is correct only for the hydrogen atom.

The basic formula describing the allowed energies of ALL electronic levels (respectively, and all

orbitals) and used for any atoms has long been obtained by quantum mechanics and is well known:

$$E_n = -\frac{hcRZ^2}{n^2}, \qquad (1)$$

где eZ - nuclear charge, an - principal quantum number [23].

The sign in the formula stands minus, as is customary in semiconductor physics, but traditionally ionization potentials are depicted as positive, which separates chemical and some physical letters of the type of solid-state physics. Adhering to the correct sign in Formula 1 and putting the world's constants equal to unity, one can construct a graph of the dependence of the energy of each allowed (according to the main quantum number n) energy level of the electron E_n on the atomic nucleus charge (Fig. 17).



Fig. 17: Dependence of the energy of allowed electronic levels (in conventional units) on the atomic number in linear (a) and double logarithmic scale (b). Pink dots show the maximum filled levels (within the framework of the elementary model). Red crosses and blue triangles show normalized reference data on the first ionization potential I_{f} / I_{f}^{H} and the work function φ / I_{f}^{H} .

In order to avoid confusion, I note at once that the generally accepted term "first ionization potential $I_{n,"}$ refers to the minimum excitation energy of an electron of an atom i.e. to the most highly filled level E_n . So I_n relates to the first quantum n = 1 only for the first period, for the second period I_n refers to the level with n = 2. And so on, the electrons of the atom tend to occupy an energetically favorable state at the allowed energy levels, i.e. the filling of levels by electrons begins with the deepest, first, then second and so on up to the total number of electrons equal to the atomic number on (in Fig. 1b the pink lines and points are E_n^{*} in accordance with the experimental period, pink circles - E_n^{*} in accordance with the model of the hydrogen-like atom).

But each level of electron energy resolved (the main quantum number) corresponds to a different number of allowed states of the electron, distinguishable

both in spin-2 and in orbital quantum number- $\{l=0,1,2,...n-1\} \Rightarrow k=n$ and in terms of the magnetic quantum number having the number of values determined by the chosen orbital number $\{m_l = l, l-1, ... - l\} \Rightarrow r = 2l + 1$ (c taking into account the spin-the placement of two electrons on the level, the number of states doubles and by additional quantum number-states). So the filling of the levels with the increasing principal quantum should go stepwise, as shown by the pink dots in Fig. 1b.

However, as can be seen from Fig. 1, the basic model of a hydrogen-like atom widely used (in introductions) gives the level filling by electrons (pink dots) qualitatively different from reality (red crosses and blue triangles in Fig. 1b). The observed first ionization potentials of atoms demonstrate that the energy of the top-filled allowed atomic level for $Z_a >> 1$ (for long periods) does not increase by orders of magnitude, as would follow from the hydrogen-like model (pink dots in Fig. 1b).

In this case, for the second "elementary" period, the number of elements is 10, which is in full accordance with the model. In addition to filling two sstates. we have two more orbital numbers $n = 2 \Longrightarrow \{l = 0, 1\}$ and, correspondingly, four additional allowed states of the electron,

$$\{l=0, m_0=0\}, \{l=1, m_1=1, 0, -1\}, \{l=2, m_1=2, 1, 0, -1, -2\} \Longrightarrow 1+3+5$$

the allowed states of electrons (pink circles in Figure 1b violation, taking into account spin-eighteen).

This long-known violation is simply accompanied by words about the greater difference in energy levels within the period than between periods. But this difference is so great that it casts doubt on the very expediency of using the calculations of the electron orbitals of large atoms based on the nucleus of the hydrogen atom.

So a completely filled s-p-hybridized electron shell of neon is similar to a completely filled s-shell of helium, and neon itself with a partially shielded nucleus is similar to helium. In general, the weakly increasing course of the first ionization potential observed in Fig. 17b qualitatively differs qualitatively from the model, which decays quadratically. It is more qualitatively more accurate to describe each period using its quasinucleus, a core shielded by internal and external electron shells. Moreover, the shape of the outer orbitals calculated on the basis of a bare core, as will be shown in the next section, can in no way be used as the first approximation for describing the crystal structure.

So when using the bare nucleus to describe the atom already in the third period, the formalism itself is violated even in the number of states. And one can use formalism only where the amendments to it are small. And they are not small, as can be seen from Figures 1 and 2, already in the second period.

Of course, there are quantitative differences already in the first period, but there are few points for analyzing the regularity. So, let's take a closer look at the "informal first" period - the second.

The analysis of quantitative differences in the second period gives an understanding that the elementary model for each period has its own "reference point" at approximately the same energy level (see $I_{\star}/I_{1}(H)$ and $\varphi / I_{1}(H)$ in Fig. 1b), and not quadratically decreasing. Therefore, the main attention was paid to a careful analysis of the quantitative differences between the elementary model and the experimental data of this period, the "elementary" and the base for more complex periods (Fig. 18).

 $\{l = 0, m_0 = 0\}, \{l = 1, m_1 = 1, 0, -1\} \Longrightarrow 1+3$ and taking into account the spin, eight (points in Figs. 1b and 2 are the normalized first ionization potential).

But already for the third period there is a difference and the number of filled states from their number, which follows from the base model. The number of elements in the third period, as well as in the second period, corresponds to the filling of four allowed electron states, rather than nine model states

for
$$n = 3 \Longrightarrow \{l = 0, 1, 2\}$$
,



Fig.18: The progress of the upper filled state E_n (pink dots is at the top and the pink dotted curve is from below) from the model dependence of the energy E_n on the atomic number and the lower figure is the experimentally observed dependences on the atomic number of the first ionization potential I_n , the work function φ and the electron affinity χ (the data contradicting the definition of affinity are represented by a dotted line).

As can be seen from the lower figure 2, all reliable data on the work function and electron affinity correlate well with the first ionization potential. In this case, the first ionization potential decreases not monotonically, but has two characteristic discontinuities. The first at the beginning of the p-orbit filling determines the s-p-splitting $\Delta_{g,p}$, the second jump is observed when the p-orbital filling begins with the electrons of the opposite spin and determines the spin splitting of p-levels Δ_{gpin} .

Therefore, it follows from the foregoing that for the third period the helium quasi-atom model also gives the correct length of the period. And the model following from the analysis of the second period, it is possible and it is necessary to use as base model. Instead of using the "through formalism" of a hydrogen-like atom with a level energy that depends only on the principal quantum number.

Moreover, the electronic structure of the elements of the second period clearly demonstrates the regular dependence of the energy of the electron levels on the additional quantum numbers (Fig. 2), and in a slightly modified form these regularities of filling the levels of the second period are almost completely repeated for the third period (in spite of the elementary model having the same number elements, as well as the second period), and the main ones are observed for all subsequent periods (Fig. 17b).

Namely, the first ionization potential of the second period does not have a monotonous dependence on the atomic number of the element (in accordance with the elementary model), but three, clearly expressed regions. The period begins with the filling of the s-orbitals first with one and then with the second electron with the opposite spin. As far as the spin of the second s-electron itself raises the second level qualitatively (by deviation from the ideal model for the first period of the core already shielded by the sshell), it is difficult to determine, since and the first slevel is not lower, but above the corresponding s-level of hydrogen.

But when going to p-levels - further filling, a characteristic jump is seen, indicating that the orbital quantum number raises the energy of the level allowed by the principal quantum number. Those, already at the atomic level there is an s-p-splitting. The filling of the p-level by the first three electrons of one spin again goes in qualitative agreement with the ideal dependence on the atomic number (the yellow band in the lower Fig. 2). But the filling of the p-level by the next three electrons of the opposite spin again begins with a jump, but continues in qualitative accordance with the ideal dependence on the atomic number of the element. That is, in addition to the traditionally considered s-p-splitting, there exists and is observed at the atomic level spin splitting.

Conducted analysis of the conformity / noncompliance of an ideal model with experimentally observed regularities allows us to make a number of fundamental amendments and conclusions.

- 1. The larger size of the screened (by internal electron shells) nucleus-quasidron raises (significantly) the allowed (near the quasinuclear) energy level for the external electron.
- 2. For the third period, the maximum orbital number remains equal to unity, as for the second period, i.e. this is a quasi-second period with "n" = 2.
- Only for the fourth period does the orbital quantum number reach 2 and d-shells arise, i.e. period with quasi- "n" = 3.
- 4. For the properties of materials, the nearest, first unfilled level-the broadening of the electronic levels-their transformation into bands also determines the metal, semiconductor or dielectric properties of the resulting materials. But for barrier effects, this is not enough a significant difference in the work function from affinity to electron not only in dielectrics and semiconductors, but also in metals directly indicates that the broadened first unfilled level does not reach the level of vacuum (zero). It follows that in the nano-size barriers the maximum height of the barrier is determined by the second unfilled level, which also manifests itself in the electron affinity.

Carbon and its dielectric analogue of boron nitride refer specifically to the second period, which determines their elementarity for a whole class of more complex materials. As can be seen from the lower figure 2, carbon also has on the upper shell two s-electrons with different spins and two p-electrons with identical spins and boron nitride, too, only on average per atom two p-electrons with exactly the same spins, since the spins of the p-electrons of the thief and nitrogen are the same. This is the similarity of the C & BN atomic orbitals and determines the similarity of their crystalline orbitals and many properties, which makes it possible to construct a base element model for most complex chemical elements. So carbon not only spawned life. Most of the other chemical elements are made in its image and likeness. its electronic structure, in principle, is preserved, only scaled.

Also, one more general statement follows from the dependence of the first ionization potential in the second and third periods. The above-mentioned spin splitting, in principle, violates the Pauli principle, which, by and large, requires registration in Fermi-Dirac statistics (and most likely in Bose-Einstein statistics). This, of course, goes well beyond the work on C & BN. Therefore, I only note that these statistics work well in solid bodies, where, as noted above, the atomic repulsion of opposite spins can be offset by the spatial separation of their electron carriers (as analyzed in the framework of the ballistic model - see the article with the same name on the site Nanotechnological Society of Russia [52] and in the book "Refinement of basic physical models" [51]).

IV. Zone Structure And Potential Barriers On The Boundary Of Two Materials

When creating semiconductor devices, the main parameter of the material is the width of the forbidden zone. At the same time, when creating interfaces, the work of the output was not given much importance. The potential barriers at the boundary for semiconductors of the same type were also determined by the width of the forbidden band. But for dissimilar materials, the magnitude of the potential barriers was an order of magnitude smaller than the difference in the work yields of the contact materials of the plates, and as a result, they believed it did not correlate with it in any way. When creating semiconductor structures for local thermo-EMF, this issue had to be given special attention [52].

As can be seen both from the general figure 1 and from the more detailed figure 2 (lower), the work function of metals clearly correlates with the first ionization potential, and for silicon depends on the type of its conductivity, ie, it correlates with the top of the valence band and bottom of the conduction band. This correlation is determined by the fact that the work function corresponds to the ceiling of the allowed zone (the blue band in Fig. 19) formed from the level of the first ionization potential I_{f} .



Fig. 19: The scheme of the appearance of allowed and forbidden zones and the internal work function of **ð** at the boundary of different materials.

As noted earlier, the first ionization potential I_7 corresponds to the maximum electron-filled level of the resolved level, and for the second period shown in Fig. 19 this is the second level in the principal quantum number: : n=2. Qualitatively, for each chemical element, being tied to its I_7 , it is possible to estimate the position of the nearest to the filled, free allowed level by the formula 1.

To this level, for n=3, whose energy is 4/9 · I_7 , there is a corresponding band of the color of the sea wave - a band of free states, a valence band, which is also present in metals, but overlapping with the band of filled states. The asymmetry specified by the polarity of the boundary leads to an external work function φ and to the external photoelectric effect at the boundary with the vacuum, and to the inner work function δ and to the internal photoelectric effect at the interface of the two materials. wave functions of empty levels of different materials on the boundary overlap.

Since the internal work function is generally unequal to zero, it follows that the energy widths of the bands of allowed states are much less than the difference between the level I_{f} and the corresponding

external work φ . So in this case, due to the crystalline interaction, there is a rise in the level filled with electrons, and the energy gain necessary for the appearance of the condensed state is apparently connected with the interaction of the nuclei with each other, which on the state of the external electrons only appears as compression and extrusion onto the surface. It is more correct to say, as was shown above, with quasinuclear interaction, which leads to a fundamental difference in the experimental characteristics obtained from the hydrogen-like atom model shown in Fig.17.

In order not to overload Fig. 19, there is no strip on it - the dependence on the atomic number of the following free states: n=4. The ceiling of this band correlates well with the experimental values of the electron affinity χ . Levels corresponding to quantum numbers greater than 4 are condensed near the vacuum level (Fig. 17), and the corresponding zones merge (the pink region on the inset showing how electrons flow across the vacuum boundary and the boundary with another material).

The circuit shown in Fig. 19 can be said to be a working scheme for microcracking of semiconductor

structures with highly effective local thermo-EMFs [18-24].

V. Analysis Of The Orientation Of Hybridized Atomic Orbitals

Logarithmic relativity is a general physical phenomenon [9], which manifests itself not only in the energy of allowed electronic states (formula 1), but also in the form of their orbitals - the electron density distribution in various allowed orbits. And quantum mechanics using a hydrogen-like model, not only counted the energy of allowed electron states to an unlimitedly large principal quantum number, but a huge number of orbitals corresponding to additional quantum numbers. But even with the example of allowed electron energies, it was shown that approximations to infinity without taking logarithmic relativity give an error greater than the base value in the zeroth approximation. Therefore, we restrict ourselves to considering only the shape of the first two orbitals, which correspond to the second period of interest to us: one s-orbital and three p-orbitals (Fig. 20a).

The s-orbit is spherically symmetric and does not impose any restrictions on the orientation of the interatomic bonds, while the three resolved p-orbitals are orthogonal and thus ALLOW and the interatomic bonds are only orthogonal, which corresponds to the elementary unit cell in the form of only an elementary cubic (Fig. 20b).



Fig. 20: The set of atomic orbitals of the second period (a) and the corresponding elementary translational cell (b) obtained in the framework of the simplest model.

If we assume that when a chemical bond is formed by an unfilled electron, one p-orbit can be neglected, then the same graphite would form a square grid of atoms. This is not observed in nature - the carbon grid is formed by hexagons.

And since chemical orbitals in both micromolecules and macro crystals can differ substantially in orientation and in shape from the calculated atomic orbitals in general, then their hybridization has been invented.

As a matter of fact, hybridization introduced to describe interatomic interactions was attributed directly to a separate atom, which means that the correction for the corrected orbitals (depicted in Fig. 20) is actually calculated, taking into account the macroscopic properties of matter from these atoms.

In fact, such an approach was a refusal to use atomic orbitals. So Pauling drew his model of sigma and pi-electrons (Fig. 21), directly contradicting the ALLOWED (resolved) atomic orbitals of graphite.



Fig. 21: Pauling fit the chemical orbitals (actually macroscopic) under the atomic idealized model (in fact, the terminology).

In principle, it was a beautiful attempt to look into the unknown microcosm. And in itself this attempt to look into the unknown, deserves the Nobel Prize, because she encouraged many chemists and physicists to do this kind of design, including me.

But already in these basic drawings it is clear that the developers (Pauling himself soon realized that the design is contradictory) is "hidden behind the thought": the diversity of the image of the links of the same size (between the nodes and the pi-link, the distance is also intra-planar \boldsymbol{a} , just like this Naturally, as between the nuclei of the sigma bond), and the "equality" of the size (represented) of the p- and s- orbitals, and the translational smearing of the π -

electrons (in contrast to the σ -electrons rigidly fixed between the nuclei).

And the "hidden" blurring of one of the four electrons (true, on both sides of the layer!)Was attributed: both the sliding of the layers along each other, and the high electrical conductivity along the layer, and for one and Van der Waals interaction between the layers. And the atoms of a single layer "liberated" by blurring would seem to be placed anywhere relative to the atoms of the other layer, but from "caution" they drew them (Fig. 22) located strictly above each other (so that all the maxima of the diffused π -bond of the neighboring layers coincide).



Fig. 22: Erroneous, but originally included in the letters, and still redrawn by many, including Wikipedia, and graphenologami, the basic model of the crystal lattice of the hexagonal phase C & BN (with the replacement of equivalent balls for graphite).

In terms of promoting understanding of the meaning of true rather than idealized allowed atomic orbitals, many results of structural and IR spectral studies were obtained in the growth of pyroxymes of graphite and boron nitride, which, in many ways, supplemented each other [7 - 12]. The closeness in energy of the upper p-orbital of carbon $(2p^2)$ to the average value of the energies of the upper half-filled p-orbitals of boron (2p) and nitrogen $(2p^3)$ indicates the similarity of external orbitals of boron nitride to carbon orbitals.

Those. the flow of an electron from nitrogen to boron leads, as it were, to the formation of two carbon atoms, only one little (as seen from the spectra of the lattice reflection BN) is positively charged and the other negatively. The polarity of the boron nitride molecule made it possible to analyze the interatomic bonds in the crystal lattice, which is practically identical to the graphite lattice in all phases, including the one depicted in Fig. 5, which demonstrates the discrepancy between the Powling orbital and not only the hexagons in the layer, but also the observed translation periods across the layers C & BN. The model of the crystal structure of the hexagonal phase, drawn by the Pulling method, gives a transmission period that does not exist in hexagonal graphite and is equal to one interplanar distance (in the experiment it is at least doubled in 3D graphite), and in hexagonal boron nitride there is such a period, and the atoms of adjacent layers are not located as in Fig. 22.

In general, the above-mentioned cycle of complex studies allows us to state that the true atomic orbitals of C & BN are inscribed, in strict accordance with symmetry, in the tetrahedron depicted in Fig. 6 (and, as studies have shown, in strict accordance with the four are involved in molecular bonds in C & BN electrons).



Fig. 23: The orientation of the true hybridized atomic orbitals C & BN.

The deformation of the atomic orbitals shown in Fig. 23 requires additional energy, which is released during the chemical reaction. However, a large deformation of atomic orbitals requires a large expenditure of energy. Therefore, the formation of chemical orbitals is more probable with a slight change in the orientation of the atomic orbitals.

Therefore, the correct, and not artificial, type of Pauling's constructions is essential, their representation is in first approximation (rather than making numerous corrections to the ideal model, or drawing them not on the basis of the principles of physics, but based on empirical data).

The atomic orbitals shown in Fig. 6 correspond directly to the crystalline orbitals of the cubic C & BN phase and only slightly deform in their other phases.

The analysis shows that it is the model of the carbon atom that should be used as the base for many chemical elements, and also for the correct description of organic life.

VI. THE REAL CRYSTAL STRUCTURE OF C & BN

The complex research carried out by C & BN touched on a number of the most general issues of the formation of atomic-molecular bonds. And a direct confirmation that the results of the analysis are true and useful are the obtaining of perfect pyrocrystals and the construction of the rhombohedral C & BN structure (Fig. 24) on the basis of the orbitals depicted in Fig. 23 and the identification of the order-disorder transition upon its transition to the hexagonal phase.



Fig. 24: The simplest, but taking into account the displacements of the atoms Δ from the plane perpendicular to the C axis (shown in the figure to the right by small arrows) is the lattice model of the rhombohedral C &BN : a - in the plane perpendicular to the C axis, b - in the plane of the section parallel to the C-axis (indicated in both figures by a dotted red line).

Three of the four orbitals depicted in Fig. 23, overlapping with the orbitals of neighboring atoms form

very rigid bonds and form the grid of hexagons depicted in Fig. 24a. The fourth atomic orbital of one monoatomic

Global Journal of Science

2018

layer "can find" an analogous orbital from the adjacent layer, but their overlap will be somewhat less because of partial rectification in the plane of the three orbitals involved in the grid of hexagons.

Figure 24b shows the cross-section of the lattice by a plane parallel to the C axis and passing along the sides of a part of hexagons. The interlayer bonds shown in Fig. 24b, which are about one and a half times less rigid than the intralayer ones, can satisfy spatial translation and form a regular lattice from the two-dimensional net of hexagons by the only method depicted in Fig. 7b, which leads to the formation of the rhombohedral phase.. These interlayer bonds provide up to about 1000 ° C the existence of a regular rhombohedral phase [6]. But since their stiffness (and,

accordingly, the Debye temperature along the C axis) is about one and a half times lower than the stiffness inside the layer bonds, then at higher temperatures, while maintaining ordering in the planes, the interlayer bonds are destroyed. This leads to a one-dimensional solid-state order-disorder transition in the hexagonal phase [11, 12]. So the hexagonal phase existing at room temperatures is metastable (hardened like the same diamond) and has ordering of interlayer bonds of the soliton type, which leads to the formation of smalldiameter crystallites. In fact, it is the interlayer bonds that form the fullerenes, and the destruction of their regularity leads, with the integrity of hexagons, to the formation of a small concentration of defects (Fig. 3) in the rhombohedral phase of the C and BN pyrocrystals.



Fig. 25: The model for the formation of the interlayer defect in C & BN.

On the left, there is a schematic representation of a 3-dimensional ordered lattice, to the right of a defect, a violation of the alternation of the direction of one interlayer bond (isolated), leading to local distortion of the monatomic layer and destruction of the spatial correlation of monolayers (the red dotted line shows the probable "erroneous interlayer bond and the unlikely" erroneous " layer bond).

The section shown in Fig. 25 demonstrates how, in principle, the interlayer bonds of the same layer can be closed to each other when one of them is passed. This is how the fullerenes are formed from which crystallization centers are formed, a large number of which lead to the formation of poorly ordered pyrocrystals from sprouting growth cones (Fig. 2).

And most of the published data refer to the type shown in Fig. 2, C & BN samples, in which many properties are determined by large intercrystalline scattering. Whereas our conclusions are based on the results of the measurement of the most perfect samples (Fig. 5a). Measurements of lattice vibrations in rhombohedral nitride of boron and measurement of plasma oscillations in rhombohedral graphite have unambiguously confirmed the asymptotic behavior of the dependences of the numerous C & BN parameters on the degree of their ordering-there is an ion-covalent bond between monoatomic layers.

The maximum of the anisotropy of C & BN is achieved on highly ordered polycrystalline hexagonal samples (Fig. 5c) and decreases, first, as the dimensions of the hexagonal crystallites increase (Fig. 5b), and then on going to the rhombohedral single crystal (pc.5a)

VII. THE BEGINNING OF THE QUASINUCLEAR MODEL

a) Inert gases are quasinuclearof periods

An atom with a quasinuclear "has" a charge equal to the number of external electrons, and the size

2018

of the quasinuclear is determined by the orbits of the inner electron shells. But screening of the core reduces its effective charge, which can be calculated using formula 1

$$E_n = -\frac{hcRZ^2}{n^2} \Leftrightarrow -\frac{hcRZ^{*2}}{n^2} = E_n^{Exp} \quad (2)$$

Thus, putting the screening factor of the hydrogen nucleus equal to unity, we obtain the screening coefficient for the helium nucleus and subsequent elements of the second period

$$k_{He}^{Z} = \frac{Z^{*}}{Z} = \sqrt{\frac{E_{n}^{*}}{E_{n}}} = \sqrt{\frac{1,8081}{4}} = 0,6723$$
⁽³⁾

Thus, the quasinuclear potential is modified for the second period, which determines the allowed energy levels of the external electrons and, in accordance with the experiment, raises them above the corresponding levels obtained from the hydrogen-like model.

At the end of the second period, we obtain, similarly (see Fig. 17), the screening coefficient for the nucleus of neon

$$k_{Ne}^{Z} = \sqrt{\frac{1,5862}{25}} = 0,2519$$
 (4)

And in accordance with the algorithm used to construct the dependence of the energy of the upper filled level in Fig. 1, we can calculate the screening coefficient for the argon nucleus

$$k_{Ar}^{Z} = \sqrt{\frac{1,1592}{36}} = 0,1794 \tag{5}$$

and all subsequent shielding ratios of inert gases.

The increase in the size of quasinuclear should also be taken into account when constructing true orbitals. As well as the features noted above, leading to a nonmonotonic dependence of the first ionization potential within the periods. But this paragraph is not accidentally called "beginning", tk. the obtained estimates of the screening coefficient of the nuclei only modify the model of the hydrogen-like atom - they adjust the basic parameter in the first approximation to the experiment. So, for the time being this is just a compilation done to examine the key moments of the proper quasinuclear model, to which, strictly speaking, the s-p-d-f-classification of electron shells is not applicable. The obtained estimates show that it is required to find true quasinuclear "originally hybridized" orbitals of the atom, like, 4 external electrons C & BN.

VIII. BIOLOGICAL ASPECTS OF THE ANALYSIS OF ATOMIC-MOLECULAR BONDS

I believe that it is not a secret that some important moments fall out of modern medical science. And only individual physicians-personalities such as Professor Shabalov (like Einstein in physics), maximally owning and modern medicine, and taking into account SOMETHING, are able to find elementary solutions when an ordinary doctor says: Modern medicine is powerless!

Another example, not for anyone, it's not a secret that not all medications prescribed by doctors lead automatically to a person's recovery. Moreover, many medications help a person purely psychologically, at the placebo level. And when creating active drugs, the principle of Hippocrates: DO NOT HAVE, as you know, is not always observed, say, in chemotherapy. So in pharmacology, we often have only attempts to follow this principle, and for a positive active intervention, both the doctor and the patient have to use a purely empirical method of trial and error.

So, medicine needs to be raised to a new level, but this requires understanding: What are the "bricks" used by it from the conjugated sciences to clarify? Of course, it also affects the fact that the organization of modern science and medicine in general is imperfect in particular, especially in modern Russia. But it is also obvious that modern science does not take into account any fundamental points. A change in the medical "brick" will not only manifest itself on the treatment of an individual directly, but due to a dynamic fractal connection, the medical "tree" itself will change.

And to "see" this "brick" we must remember that life on Earth is organic and its main brick is carbon. So the formation of "molecules of life" - cells is determined primarily by carbon. And not by chance, tk. it is the carbon fullerenes that are part of a chemical chain reaction that disrupts normal statistics, preserving information about the past, and thereby accelerating the development of the processes, makes the probability of the occurrence of life nonzero. Carbon fullerenes are cosmic sperm that has taken root in the "womb" of the Earth. Therefore, it is necessary to take into account the properties of carbon in the first place, whereas modern pharmacology deals primarily with catalysts - other chemical elements and their compounds.

Physical concepts of the electronic structure of carbon, were laid by the chemist Pauling to explain the anisotropy of graphite [1]. Practically in their original form they are still preserved, both in physics itself, in chemistry, and in their special directions, in particular in pharmaceuticals. Although Pauling himself tried to eliminate the contradictions in his model by introducing "curved chemical bonds," but the further development of science followed the original track he laid [2]. So that to curtail from this gauge it is required taking into account modern knowledge to consider more thoroughly both the chemical bonds of carbon, and chemical bonds in general, tk. at their construction in an implicit kind were repelled from representations from chemical communications of carbon.

The fact that carbon has become in implicit form the basis for general ideas about chemical bonds, as will be shown in the article not by chance. Therefore, the refinement of its electronic structure is important not only for a correct analysis of the structure and properties of organic matter, but also for the electronic structure of most chemical elements and for the properties of materials [3], including those used in medicine.

IX. Conclusion

Any model, in principle, has limits of applicability. The widely used model of a hydrogen-like atom, as shown in this paper, is qualitatively broken already in the second period, and for the following periods gives a catastrophic discrepancy with the experimental data.

The complex study of C & BN pyrocrystals not only clarified their crystal structure and properties, made it possible to obtain perfect pyrocrystals and, on their "elementary" basis, to make a qualitatively new "brick" for the construction of atoms, namely their electronic orbitals.

Thus, it has been shown that even in the simplest chemical compounds, even in the "elementary" carbon atom, it is required to refine the concepts of the strength and form of atomic-molecular bonds. At the same time, it is possible and necessary to build models of atomic-molecular bonds of many chemical compounds on the basis of an "elementary", but more complex than a hydrogen atom, a carbon atom.

References Références Referencias

- Pauling L. "Nature of the chemical bond" / under. Ed. Ya.K.Syrkin. - M.-L .: The Publishing House of Chemical Literature, 1947. 440 p.
- 2. F. Bassani, J. Pastori-Parravichini "Electronic states and optical transitions in solids", Moscow, 1983, Nauka, 392 p.
- Grigorovich VK, "Mendeleyev's Periodic Law and the Electronic Structure of Metals", Nauka Publishers, Moscow, 1966, 288 p.
- S.V. Ordin, [B.N. Sharrupin], J. Semiconductors (FTP), 32(9), 924-932, 1998, Normal Lattice Oscillations and Crystalline Structure of Non-Isotropic Modifications of a Boron Nitride. (С.В.Ордин, Б.Н.Шарупин, М.И.Федоров, ФТП, 1998т., 32, №9, с.1033.)
- George . Pimentel, Richard D. Spratley, @Chemical bonding clarified through Quantum Mechanics", HOLDEN – DAY, INC, Cambridge, 1970, 332 pp.

- Ordin S.V., Ballistic model of the movement of electrons over potential hill, PHTI of A.F.loffe of the Russian Academy of Sciences, St.-Petersburg, Russia, Interstate Conference: Thermoelectrics and their application, on November, 2014, Proceedings, St.-Petersburg, Russia, 2015, p.199-203, http://www.rusnor.org/pubs/articles/11583.htm
- Stanislav Ordin, Book: "Refinement of basic physical models", Lambert, 2017, Project № 163273, ISBN: 978-3-659-86149-9, 82 pp.
- Ordin S.V. "So is there a NANO science?" J. NBICS: Science. Technology. Vol. 2, No. 3, pp. 77-87, 2018. http://www.rusnor.org/pubs/articles/ 15519.htm
- 9. S.V. Ordin, Logarithmic relativity, 2017, http://www. rusnor.org/pubs/articles/15503.htm
- S.V. Ordin, "Giant spatial dispersion in the region of plasmon-phonon interaction in one-dimensionalincommensurate crystal the higher silicide of manganese (HSM)", Book: Optical Lattices: Structures, Atoms and Solitons, Editors: Benjamin J. Fuentes, Nova Sc. Publ. Inc., 2011, pp. 101-130.
- B.N. Sharupin "Structure and properties of boron pyronitride", in the book. Ed. V.S. Shpaka and R.G. Avarbe "Chemical gas-phase deposition of refractory inorganic materials", 1976, Leningrad, GIPHH, 104 p.
- S.V.Ordin, M.I.Fedorov, V.I.Rumyantsev, E.V.Tupistina, A.S.Osmakov, Crystal Structure and Anisotropy of Luminesence of Rhombohedral and Hexagonal Phase of Boron Nitride, Abstracts of MRS, 1998.
- 13. S.V.Ordin, CRYSTAL STRUCTURE AND ANISOTROPY OF LUMINESENCE OF RHOMBOHEDRAL AND HEXAGONAL PHASE OF BORON NITRIDEA.F.IoffePhysico-Technical Institute of RAS, St. Petersburg, RUSSIA; B.N. Sharrupin, "ROMBONIT" Ltd., St. Petersburg, RUSSIA; M.I. Fedorov, A.F.IoffePhysico-Technical Institute of RAS, St. Petersburg, RUSSIA; V.I. Rumvantsev, E.V. Tupitsina, A.S. Osmakov, "ROMBONIT" Ltd., St. Petersburg, RUSSIA. MRS-SYMPOSIUM I, III-V and SiGe Group IV Device/IC Processing Challenges for Commercial Applications December 2 - 3, 1998 Chairs p. l2.11
- Ordin S.V., Rumyantsev V.I., Tupitsina E.V., Osmakov A.S., Avdeev O.V., Fedorov M.I., Features of Band Structure and Seebeck Coefficient Anisotropy of Pyrographites, Proceedings of VI Interstate Seminar: Thermoelectrics and their applications, October, 1998, St.-Petersburg, Publishing House of the Russian Academy of Science, 1999, p. 123-130, p.278-279.
- 15. Ordin S.V., Osmakov A.S., Rumyantsev V.I., Tupitsina E.V., Shelyh A.I., Features of an electronic spectrum and a microstructure of graphite, IX National conference on growth of crystals (NCCG

2000), theses of reports, Moscow, Crystallography Institute of the Russian Academy of Science, 2001, p.53.

- Ordin S.V., Rumyantsev V.I., Tupitsina E.V., Osmakov A.S., Real structure and transition of type the order–disorder in modifications pyrolitic boron nitride, IX National conference on growth of crystals (NCCG 2000), theses of reports, Moscow, Crystallography Institute of the Russian Academy of Science, 2001, p.57.
- 17. Ordin S.V., Osmakov A.S., Rumyantsev V.I., Tupitsina E.V., Shelyh A.I., REAL STRUCTURE AND TRANSITION OF THE ORDER-DISORDER TYPE IN MODIFICATIONS OF PYROLYTIC BORN NITRIDE, Surface, X-ray, synchrotron and neutron researches (Moscow) 5, 108, 2003. (РЕАЛЬНАЯ СТРУКТУРА И ПЕРЕХОД ТИПА ПОРЯДОК-БЕСПОРЯДОК В МОДИФИКАЦИЯХ ПИРОЛИТИЧЕСКОГО НИТРИДА БОРА, Поверхность, 2003, №5, с 108.)
- S.V. Ordin, W.N. Wang, "Thermoelectric Effects on Micro and Nano Level.", J. Advances in Energy Research, Volume 9, 2011, p.311-342.
- 19. Ordin S.V., Announcement of the book «Structure and properties of C & BN - extremely anisotropic crystals».http://www.rusnor.org/pubs/articles/15602. htm
- Ordin S.V., American Journal of Modern Physics, Refinement and Supplement of Phenomenology of Thermoelectricity, Volume 6, Issue 5, September 2017, Page: 96-107, http://www.ajmp.org/article? journalid=122&doi=10.11648/j.ajmp.20170605.14
- Ordin S.V., "Cardinal increase in the efficiency of energy conversion based on local thermoelectric effects", International Journal of Advanced Research in Physical Science, Volume-4 Issue-12, p. 5-9, 2017. https://www.arcjournals.org/internationaljournal-of-advanced-research-in-physicalscience/volume-4-issue-12/
- S. V. Ordin, Yu. V. Zhilyaev, V. V. Zelenin, V. N. Panteleev, Local Thermoelectric Effects in Wide-Gap Semiconductors, Semiconductors, 2017, Vol. 51, No. 7, pp. 883–886. DOI: 10.21883/FTP.2017.07.44643.29
- S.V. Ordin, "Experimental and Theoretical Expansion of the Phenomenology of Thermoelectricity", Global Journal of Science Frontier Research- Physics & Space Science (GJSFR-A) Volume 18, Issue 1, p. 1-8, 2018. https://globaljournals.org/GJSFR_Volume 18/E-Journal_GJSFR_(A)_Vol_18_Issue_1.pdf
- S.V. Ordin, «"Anomalies in Thermoelectricity and Reality are Local Thermo-EMFs», GJSFR-A Volume 18 Issue 2 Version 1.0, p. 59-64, 2018 https://globaljournals.org/GJSFR_Volume18/6-Anomalies-in-Thermoelectricity.pdf
- 25. J. W. McClure, «Band Structure of Graphite and de Haas-van Alfen Effect», Phys. Rev., 108, 3, (1957), p.612-618.

- 26. I.C.Slonczewski, P.R.Weis. Phys.Rev., 109, (1958), p.272
- 27. У. Харрисон, Электронная структура и свойства твердых тел, М. Мир, 1983, с. 125,130,218.
- 28. Bacon G.E., Acta Crist., 1950, v.3, p.137.
- 29. М.М Ефременко, А.Е.Кравчик, А.С. Осмаков, ЖПХ, 1993, т 66, N 1, стр. 107-112.
- 30. С.В.Шулепов, «Физика углеграфитовых материалов», М. Металлургия, 1972, 254с.
- 31. А.Е.Кравчик, А.С. Осмаков, Р.Г. Аварбэ, ЖПХ, 1989, т 62, N 11, стр. 2430-2435.
- 32. By Ko Sugihara and Hisanaro Sato, «Electrical Conductivity of Grafite», J. of the Physical Society of Japan, 18, 3, (1963), 332-341.
- А. И. Лутков, «Тепловые и электрические свойства углеродных материалов», М. Металлургия, 1990,176 с.
- 34. В.С. Нешпор, Структура и физические свойства разновидностей пирографита, в кн. под ред. В.С. Шпака и Р.Г. Аварбэ «Химическое газофазное осаждение тугоплавких неорганических материалов», Ленинград, 1976, 32-65с.
- 35. Ордин С.В., Румянцев В.И., Тупицина Е.В., Осмаков А.С., Авдеев О.В., Федоров М.И., «Термоэлектрики и их применение», Доклады VI Межгосударственного семинара (октябрь 1998 г.), РАН, ФТИ им. Иоффе, С.-Пб., 1999, с. 123-130.
- 36. E.A. Taft and H.R. Philipp, «Optical Properties of Graphite», Phys. Rev., 138, (1965), A197-A 202.
- D.L. Greenoway, G. Harbeke, F, Bassani, E. Tosati, «Anisotropy of Optical Constants and the Band Structure of Graphite», Phis. Rev., 178, 3, (1969), 1340-1348.
- 38. H.R. Philipp, «Infrared optical properties of graphite», Phis. Rev. B, 16, 6, (1977), 2896-2900.
- M. S. Dresselhaus and G. Dresselhaus, «Intercalation compaunds of graphite», Adv. InPhys., 1981, 30, 2, 139-326)
- 40. J.T.Mc Cartney and S.Ergun, Optical Properties of Graphite and Coal, Proceedings of the Third Conference on Carbon, Held at the University of Buffalo, Buffalo, New York, Pergamon Press, 1975, p. 223-231.
- 41. А.С. Котосонов, «Электропроводность углеродных материалов со структурой квазидумерного графита», ФТТ, 31, 8, (1989), 146-152.
- 42. В.В. Авдеев, В.Я. Акимов, Н.Б. Брант, В.Н. Давыдов, В.А. Кульбачинский, С.Г. Ионов, «Энергетический спектр эффект Шубникова-де Гааза у гетероинтеркалированных соединений графита акцепторного типа», ЖЭТФ, 94, 12, (1988), 188-201.
- 43. C.F. Quate, Physics Today, August 1986, p.26.
- 44. Бараш Ю. С., «Силы Ван-дер-Ваальса», М., 1988, «Наука», 344с.
- 45. С.В.Попова, Н.А.Бенделиани, «Высокие давления», Москва, «Наука», 1974, 236 с.

2018

- Б.Н.Шарупин, А.С.Осмаков, Е.В.Тупицына и др., ЖПХ, т.64, №8, с.1698, 1990.
- 47. Б.Н.Шарупин, В.В.Лопатин, В.С.Дедков и др., Неорганические Материалы, 1996, т.32, №6, с. 690.
- 48. С.Н.Гриняев, В.В.Лопатин, Электронная структура графитоподобного и ромбоэдрического нитрида бора// Изв. ВУЗов, Физика, 1992, т.35, №2, с.27.
- В.А.Бутенко, В.В.Лопатин, В.П.Черненко, Неорганические Материалы, 1984, т.20, №10, с.1657.
- 50. A.Simpson, A.D.Stuckes, J. Physical Chemistry, 1971, v. 4, p.1710
- Stanislav Ordin, Book: "Refinement of basic physical models", Lambert, 2017, Project № 163273, ISBN: 978-3-659-86149-9, 82 pp.
- 52. Ordin S.V., Ballistic model of the movement of electrons over potential hill, PHTI of A.F.loffe of the Russian Academy of Sciences, St.-Petersburg, Russia, Interstate Conference: Thermoelectrics and their application, on November, 2014, Proceedings, St.-Petersburg, Russia, 2015, p.199-203. http://www.rusnor.org/pubs/articles/11583.htm