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Dedicated to the memory of B.K. Vainshtein

Tetrahedral Structures with Icosahedral Order and Their Relation to Quasicrystals

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Abstract—The possible existence of quasicrystals in tetrahedral phases is considered. It is shown that one of the well-known crystalline silicon phases (the BC8 phase or silicon III) is characterized by the icosahedral local order with three-quarters of the interatomic bonds being directed along the fivefold axes of an icosahedron. This crystal is considered as an approximant of an icosahedral quasicrystal. Higher order approximants and other tetrahedral structures related to quasicrystals are also constructed. It is shown that in these structures, the formation of the intrinsic phason disorder with the preservation of the energetically favorable coordination number four is possible. The *ab initio* quantum-mechanical calculations for carbon and silicon show that, although all the considered phases are metastable, their energies only slightly differ from the energies of the corresponding stable phases. *© 2001 MAIK “Nauka/Interperiodica”.*

INTRODUCTION

Boris Konstantinovich Vainshtein was always deeply interested in the fundamental problems of crystallography and keeping in contact with people studying these problems. Therefore, it seems to be not accidental that the first true crystallographic paper on quasicrystals entitled *De nive quinquagula* (On Pentagonal Snowflakes) was dedicated to the 60th birthday of Vainshtein and written by a friend of his, the famous British scientist Mackay, several years prior to the discovery of quasicrystals [1]. Earlier, the quasiperiodic functions and surface tilings were studied only by mathematicians [2, 3], so that nothing indicated the future revolution in crystallography which would follow the discovery of icosahedral quasicrystals in metal alloys [4]. In the following years, Vainshtein always encouraged the development of this direction at the Institute of Crystallography. He was the initiator of complementing the new edition of *Modern Crystallography* [5] with the chapter entitled *Quasicrystals*. The joint work over this chapter had become for one of the authors of this article (V.E.D.) the unique possibility of getting acquainted with the phenomenal scientific intuition and capacity for work characteristic of Vainshtein. Of course, it would have been very useful to discuss such a surprising turn in the problem of existence of quasicrystals in tetrahedral systems considered in the present article with such scientists as Vainshtein and V.L. Indenbom, but, alas, it is not possible. Thus, we can only hope that someone else would take interest in this problem.

The basic achievements of the science of quasicrystals have already been included into textbooks on crystallography [5, 6], but they all relate to quasicrystals in metal alloys. In addition to icosahedral quasicrystals [4], other quasicrystals were also discovered—octagonal, decagonal, and dodecagonal [7–9]—whose point symmetry groups included the eight-, ten-, and twelvefold rotation or screw axes, respectively. All these quasicrystals have dense atomic structures characterized by the noncrystallographic symmetry with the atoms usually being surrounded by ten to sixteen nearest neighbors in the first coordination sphere. Since there are no covalent bonds, the atoms can be considered as spheres of different diameters. In the tetrahedral structures, each atom has four neighbors related to it by directional covalent bonds (the classical example here is the diamond structure). Therefore, it is still unclear how to apply the attractive ideas of the theory of metal quasicrystals to the systems with tetrahedral coordination. This problem is closely related to the structure of amorphous substances which can also have metal or covalent bonds; this has also been exhaustively studied for many years.

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One of the most often used approaches to the problem is based on the well-known fact that there exists a class of structures characterized by high atomic density—the so-called tetrahedrally close-packed structures—that can be geometrically transformed into the structures with tetrahedral coordination. In the tetrahedrally close packed structures, all the interstitials are tetrahedral; i.e., all the atoms are located at the vertices of slightly distorted tetrahedra (see review [10]). These tetrahedra should necessarily be distorted because the three-dimensional space cannot be tiled with ideal tetrahedra. An example here is the so-called Frank–Kasper crystalline phases observed in numerous metal alloys [11]. One of the most often encountered structural motifs in these structures is an icosahedron with the coordination number of the central atom 12 (coordination numbers 14, 15, and 16 are also possible). In the tetrahedrally close-packed structures, each tetrahedron shares the faces with four neighboring tetrahedra. Therefore, performing the dual transformation (placing "new" atoms into the centers of each tetrahedron and removing all the "old" atoms), one arrives at a new structure with tetrahedrally coordinated atoms [11]. Of course, in this type of structure, the bond lengths differ from one another and the bond angles differ from the ideal tetrahedral angle $\theta_{tetr} = \arccos(-1/3) \approx 109.47°$, which is not favorable in terms of energy. One more serious drawback of these dual structures is the formation of large cavities. To the atoms with the icosahedral coordination there correspond cavities in the shape of distorted dodecahedra. Even larger cavities are formed at the atomic sites characterized by the coordination numbers 14, 15, and 16. Therefore, the average atomic density of these structures is rather low. Nevertheless, such metastable structures can be obtained experimentally, e.g., for silicon (they are related to the class of clathrate compounds).

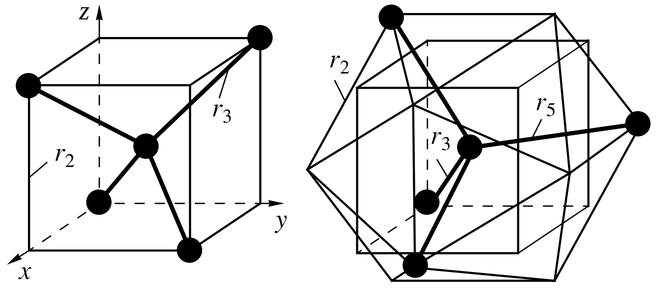
A similar approach has long been used in precomputer modeling of amorphous structures. The icosahedral and dodecahedral motifs are rather typical of the spherical models of metal glasses [12] and amorphous semiconductors [13], respectively. A more consistent theory providing the construction of both crystalline and amorphous tetrahedrally close packed structures is based on the fact that the curved space (a three-dimensional sphere in the four-dimensional space) can be tiled with ideal tetrahedra; this tiling has an icosahedral symmetry. The "flattening" of this curved space results in tetrahedrally close packed structures with local icosahedral motifs in the plane three-dimensional space, which is inevitably accompanied by the formation of specific defects—disclinations [14]. A similar construction is also possible for tetrahedral structures [15] (for details see the review articles [16, 17]).

Some icosahedral quasicrystals are also related to the Frank–Kasper phases, e.g., the Al–Li–Cu alloys. Therefore, it was suggested to apply the dual construction considered above to tetrahedral quasicrystals [18] (see also recent publications [19, 20]). Another traditional method applied to quasicrystals—the projection from a multidimensional space—showed that the attempts to construct icosahedral crystals with the coordination number four have failed and that many atoms are characterized by coordination numbers three and even two; in other words, there are too many dangling bonds [21]. Dangling bonds are also obtained in the comparatively simple decoration of the rhombohedral Penrose tiling [22]. A more sophisticated decoration of rhombohedra with dodecahedra and the related polyhedra provides the construction of quasicrystal structures with almost no dangling bonds (less than 1%) [23, 24], but, in these models, the order is formed at such long distances that they should be considered rather as models of amorphous structures.

The progress in the experimental studies of this field was considerably hindered by the absence of the so-called *approximants*—crystals with a local atomic order close to that in quasicrystals. With an increase of the approximant order, their unit cells also increase, so that their structures and properties become even more similar to those of quasicrystals. At the same time, the structures of approximants can be studied by the traditional methods of X-ray diffraction analysis. For conventional metal quasicrystals, numerous approximants are known whose structures can be determined by the standard methods. This fact provided for the rapid progress in understanding the nature of quasicrystals. Recently, it was also shown that there are quasicrystal approximants for structures with tetrahedral coordination [25]. Below, we describe in detail these crystalline phases and their specific phason-type defects.

ICOSAHEDRAL ORDERING AND THE BC8 PHASE OF SILICON

The metastable silicon phase BC8 (or silicon III) has long been known [26]. Under pressures exceeding 10 GPa, the diamond structure of silicon (silicon I) is transformed into the β-tin (white tin) structure (silicon II) structure. The removal of the pressure does not lead to the initial structure; instead, silicon II is transformed into a metastable cubic phase, silicon III, with 16 atoms in the body-centered unit cell (the lattice parameter a = 6.636 Å, sp. gr. $Ia\bar{3}$). Since the corresponding primitive rhombohedral unit cell (used in the *ab initio* calculations of the structure and the electronic properties) contains eight atoms, this body-centered cubic phase is called the BC8 phase. At room temperature, this phase is rather stable but annealing at comparatively low temperature (about 100°C) results in its transformation, first, into the hexagonal lonsdaleite-type structure and, then, into the stable diamond structure. The BC8 phase is observed for germanium; similar phases are also known for binary compounds. The articles on the "exotic phases" in semiconductors were reviewed in [27].



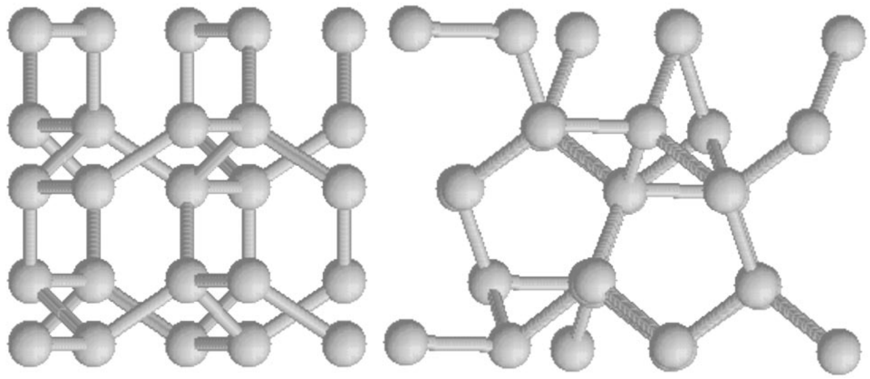
(a) (b)

Fig. 1. Illustrating tetrahedral ordering in the (a) diamond structure and (b) BC8 phase. Covalent bonds are indicated by bold lines. In the ideal structure, the icosahedron edges are exactly equal to the cube edges (for simplicity, the unseen edges of an icosahedron are not indicated). The cubes in (a) and (b) are the same, their edges are twice shorter than the lattice constant of the diamond structure and τ^2 times shorter than the lattice constant of the BC8 phase. In both cases, the center of inversion is located in the middle of the bond directed along the threefold axis.

All the atoms in the BC8 structures occupy the crystallographic position 16(c) and lie on threefold axes. This structure is well described on the Internet [28]. Only recently, was it shown [25] that this structure is characterized by the "hidden" icosahedral order—three-quarters of all the covalent bonds are directed almost along the fivefold axes of an icosahedron (Fig. 1). Each atom has two types of bonds denoted by letters A and B. The type-A bonds are directed along the threefold axes as in the diamond structure. The orientations of three B-type bonds depend on the value of the parameter x. Replacing the experimental value $x = 0.1003$ by the ideal value $x_{ic} = \tau^{-2}/4 \approx 0.0955$, where $\tau = (1 + \sqrt{5})/2$ (the so-called golden mean), one can make B bonds parallel to the fivefold axes of an icosahedron, i.e., to the $\langle 01\tau\rangle$-type directions. The motifs typical of the icosahedral symmetry can be distinctly seen only if the structure is projected along these crystallographically unusual directions (Fig. 2). The angles between the bonds slightly differ from one another, and, instead of one tetrahedral angle $\theta_{tetr} \approx 109.47°$ (as in the diamond structure), the BC8 structure has two angles: $\theta_{BB} = \arccos[(1-2\tau)/5] \approx 116.56°$ and $\theta_{AB} = \arccos(-1/\sqrt{12\tau+9}) \approx 100.81°$.

Similar to any approximant of an icosahedral crystal, the ideal structure of the BC8 phase can be obtained by projecting the points of a certain six-dimensional cubic lattice onto the real space [25, 29]. In our case, the six-dimensional lattice is a body-centered one, whereas for conventional quasicrystals and their approximants, the six-dimensional lattices are either primitive or face-centered. The lengths of the A and B bonds, r_3 and r_5, are related to the constant a_r of the quasilattice in the same way as in the conventional metal quasicrystals, $r_5 = a_r/\tau$ and $r_3 = a_r\sqrt{3}/\sqrt{4\tau+3}$. The lattice constant a_{BC8} of the BC8 phase corresponds to the lattice constant of the 1/0 approximant, namely, $a_{BC8} = a_{1/0} = 2\tau a_r/\sqrt{1+\tau^2}$ (the fact that BC8 is an approximant was first established in [22]). Thus, a_r for silicon should be about 3.9 Å. It should be indicated that another interatomic distance characteristic of quasicrystals and their approximants—$r_2 = 2a_r/\sqrt{4\tau+3}$ (this distance is equal to the edge of the cube and the icosahedron in Fig. 1)—is absent in the BC8 structure, although it cannot be excluded that it would be detected in higher order approximants. Due to the partial similarity symmetry inherent in approximants, the BC8 structure has many distances $\tau^n r_5$, $\tau^n r_3$, and $\tau^n r_2$ with $n = 1, 2$, whereas the quasicrystals can have any distances with $n > 1$.

It should be indicated that exactly the same structure for the BC8 phase can also be obtained at another value of the atomic coordinates, $x = x'_{ic} = \tau x_{ic} \approx 0.1545$, but,



(a) (b)

Fig. 2. (a) The BC8 structure viewed along the z-axis. The atoms and the bonds are shown. The maximum horizontal and vertical distances between the atoms correspond to the lattice constant. (b) The same structure viewed along the fivefold axis. One can see regular pentagons and half of a decagon, but it should be kept in mind that the structures are not planar.

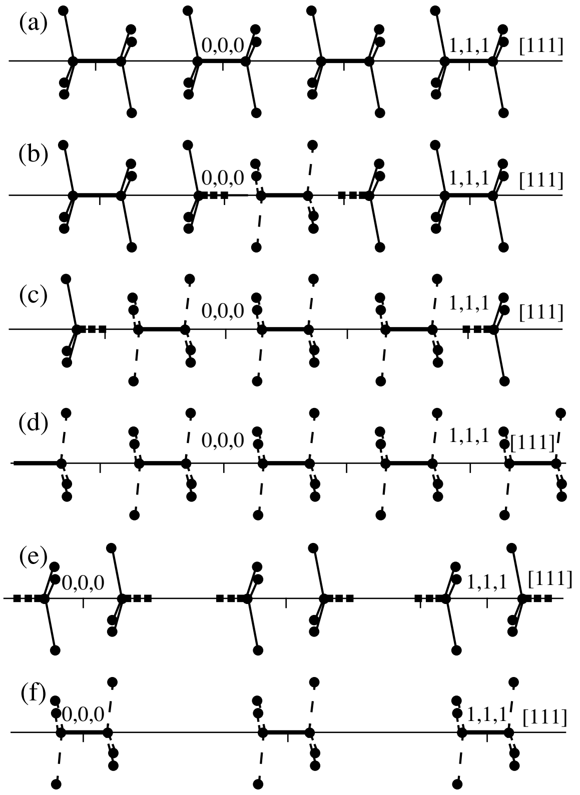


Fig. 3. Illustrating the formation of phasonlike defects in the 1/0 (the BC8 phase) and the 1/1 approximants. The A bonds are shown by bold lines; the B bonds, by solid lines; the C bonds, by dashed lines; and the dangling bonds, by bold dashed lines. (a–d) The BC8 phase; all the atoms are in the 16(*c*) positions on threefold axes. (a) The chain of atoms in the vicinity of one of the threefold axes of the ideal structure. (b) Two atoms jump toward one another forming a new A bond and two dangling bonds. (c) Dangling bonds "propagating" along the chain. (d) The whole chain is switched into a new state; there are no dangling bonds, only the A and the C bonds exist. (e, f) The 1/1 approximant; the atoms lying on the axis and outside it occupy the positions 16(*c*) and 48(*e*), respectively. (e) The initial structure with dangling bonds for the atoms lying on the axis (the atoms lying outside the axis have four bonds). (f) Annihilation of all the dangling bonds upon phason jumps.

in this case, the structure is rotated as a whole by 90° with respect to the initial structure. As a result of this rotation, all the B-bonds are oriented along the $\langle 0\tau 1\rangle$ directions and not along the initial $\langle 01\tau\rangle$ directions. It will be shown that this global rotation can be provided by local jumps of the atoms.

PHASON DEFECTS

The unique property of the BC8 phase is the possible formation of linear defects providing the preservation of the energetically advantageous coordination number of four. The corresponding process is schematically depicted in Fig. 3. The BC8 structure can be represented by chains of atoms located on threefold axes and spaced by distances r_3 (A bonds) and τr_3 (Fig. 3a). In approaching one another, two atoms spaced by τr_3 can be displaced from their sites to form a new A bond and two dangling bonds (Fig. 3b). These dangling bonds can "propagate" in opposite directions along the chain and cause small jumps of atoms and bond switching (Fig. 3c). Upon the "annihilation" of all the dangling bonds on the crystal surface or at defect, the atomic chain is switched into a new state in which the B bonds are replaced by newly formed C bonds (Fig. 3d). All the C bonds have the $\langle 1\tau^3\tau^3\rangle$ orientation and the lengths $r_C = r_2\sqrt{5\tau+6}/4$ intermediate between the lengths of the A and B bonds.

These jumps of the atoms are analogous to those observed in conventional quasicrystals and are called phason jumps, whereas the corresponding structural defects are called phason defects. Using the analogy between phonons and phasons, they are called *bondons*. This term combines the English and the French meanings of the word *bond* (bond and jump, respectively).

It is possible to show that not only one but any number of chains can be switched into new states with the preservation of coordination number four [25]. If all the chains parallel to one of the threefold axes are switched into another state, e.g., parallel to the [111] axis, one arrives at the structure described by the rhombohedral space group $R\bar{3}$ (which is a subgroup of the sp. gr. $Ia\bar{3}$). Such a switching was observed experimentally upon the change of the pressure as a reversible phase transition between two metastable phases—the BC8 phase and the rhombohedral phase R8 with eight atoms per unit cell [30, 31]. Switching of all the chains parallel to two different threefold axes generates the body-centered tetragonal structure with 16 atoms per unit cell [32]. The corresponding structure was given the name BT8, sp. gr. $I4_1/a$, with all the atoms being located in one general position 16(*f*). The energy and the powder diffraction data for the BT8 phase are close to those of the R8 phase, and, therefore, it is not quite clear which of these two phases is really observed in the experiment [32].

Switching of all the chains parallel to three different threefold axes yields the R8 structure again. If all the chains are switched, we arrive at the BC8 phase but with a new parameter x equal to x'_{ic}, which signifies that the small local jumps of atoms can result in the rotation of the structure as a whole by 90° with respect to the initial structure. If all the chains are switched chains randomly, i.e., in such a way that each chain can be found in one of the two states with the probability 1/2, then the disordered structure formed is described by the sp. gr. $Ia\bar{3}d$ and the diffraction pattern from this structure is similar to the diffraction patterns from amorphous structures [25]. Switching the chains in different ways, one can obtain an infinitely large number of ordered and disordered structures.

The *ab initio* calculations were performed for several structures of this type. The early computations and the corresponding references can be found in [27]. These quantum-mechanical computations of the equilibrium structures and the electronic properties of the crystals are quite reliable. It was shown that in silicon, all the BC8-based structures are metastable in comparison with either the diamond structure (under low pressures) or the β-tin structure (at high pressures) [32]. The energy of an isolated phasonlike defect is not too high, and therefore, it is possible to assume the existence of some number of these defects in real specimens of the BC8 phase. This should be taken into account in the structure analysis of these phases. It was also shown that the elastic properties of the BC8 phase are almost isotropic, as was to be expected for the approximants of icosahedral quasicrystals (the elastic properties of icosahedral quasicrystals are isotropic because of their high symmetry).

THE 1/1 APPROXIMANT

In addition to the BC8-based structures (i.e., the approximant 1/0), it is also possible to construct the approximant 1/1 whose unit cell exceeds the unit cell of the approximant 1/0 by a factor a τ. The space group of this approximant is also $Ia\bar{3}$; 64 atoms are located in the 16(*c*) position with $x = x_{ic}$ and the 48(*e*) position with $x = (1 - 2x_{ic})/2$, $y = (2\tau - 1)x_{ic}$, and $z = x_{ic}$. This structure is also formed by atomic chains (Fig. 3e), but it is obvious that the atoms lying on the chain axes are characterized by the energetically disadvantageous coordination number—three. However, these atoms can also perform the same jumps as in the BC8 phase, which results in disappearance of all the dangling bonds (Fig. 3f). The *ab initio* calculations for carbon and silicon show that, energetically, the approximant 1/1 is less advantageous than the BC8-based structures [32, 33]. Up to now, all the attempts to construct higher-order approximants without dangling bonds have failed.

THE A15-BASED STRUCTURES

The structures related to that of the BC8 phase are not the only structures with tetrahedral coordination, high atomic density, and icosahedral motifs. One can readily see that numerous structures of this type can be obtained from the Frank–Kasper phases using a novel approach [33].

As an example, consider one of the typical Frank–Kasper phases, the so-called A15 structure (Fig. 4a), characterized by the spatial symmetry $Pm\bar{3}n$ (eight atoms per unit cell). The atoms located in the center and at the cube vertices are characterized by coordination number 12 (a distorted icosahedron), whereas the atoms located on the faces, by the coordination number 14. All the interstitials are tetrahedral. The standard method for obtaining the structures with the tetrahedral coordination is reduced to the relocation of "new" atoms into the interstitials and the removal of all the "old" atoms. As a result, one arrives at the clathrate structure with 46 atoms per unit cell described by the same space group. The atoms in this structure form slightly distorted dodecahedra around the center and the vertices of the cubic unit cell; the density of this structure is relatively low.

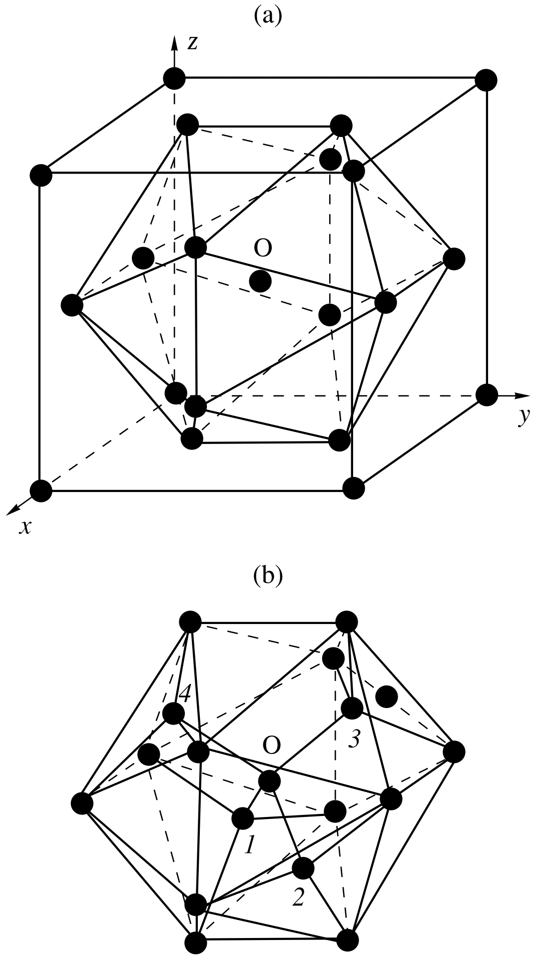


Fig. 4. (a) The A15 or V_3Si structure. Atoms are in the center and at the vertices of the cube and the icosahedron inscribed into this cube. The icosahedron is irregular, its edges are equal to the half-edge of the cube, whereas the regular icosahedron has the edge τ times shorter than the edge of circumscribed cube. The same icosahedra but rotated by 90° are located around the cube vertices. (b) The tetrahedral structure formed from the A15 structure. For simplicity, only one icosahedron with four new additional atoms (*1*, *2*, *3*, and *4*) inside it is shown; the covalent bonds are shown by solid lines.

Here, we will use another method for transforming the A15 structure into the structure with tetrahedral coordination (Fig. 4b). We leave infact all the old atoms and place a small additional tetrahedron (four atoms) located in each icosahedron. As a result, the unit cell contains 16 atoms in the positions 2(*a*), 6(*d*) (old atoms), and 8(*e*) (new atoms), and the symmetry of the new structure is described by the sp. gr. $P\bar{4}3n$. Obviously, the atoms in the center and at the tetrahedron vertices have four bonds (Fig. 4b). The atoms at the icosahedron vertices have one bond inside the icosahedron, but, since the symmetry of these positions is $\bar{4}$, each atom at the vertex has four such bonds from different icosahedra, which results in the formation of the structure in which all the atoms are tetrahedrally coordinated. All the bond angles exceed 90°, but differ from the ideal tetrahedral angle. The *ab initio* calculations show that, under reasonable pressures (attainable in diamond anvils) and zero temperature, the energy of this carbon phase is higher than the energy of diamond (by about 0.6 eV under the zero pressure) [33]. If this phase was more advantageous under high pressures and temperatures, this would have allowed one to explain the tetrahedral growth forms occasionally observed for diamonds, which gave rise to a lengthy discussion on its true structure (the tetrahedral growth forms are allowed for the $P\bar{4}3n$ symmetry).

It should also be noted that a tetrahedron can be inscribed into each icosahedron by ten different ways. Therefore, similar to the BC8 phase, this method allows the construction of an infinite number of both ordered and disordered structures. Of course, in many cases, the bond angles are acute and, thus, energetically unfavorable, but the *ab initio* calculations for carbon show that some of the rhombohedral structures thus obtained are energetically more advantageous than the cubic structure described by the sp. gr. $P\bar{4}3n$, although less advantageous than the diamond structure. This makes it necessary to perform new thorough studies along these lines.

CONCLUSION

Despite progress in understanding the structure of approximants, the quasicrystals with the tetrahedral coordination still remain purely hypothetical. However, the investigations performed provided the development of new methods for constructing both rather complicated crystalline and partly disordered structures with tetrahedral coordination. For some of these structures, it was possible to perform *ab initio* calculations and determine the exact atomic coordinates and the elastic and electronic properties. These structures can also be used for modeling amorphous carbon and silicon.

It should be emphasized that, recently, an experiment has been made in which the electron diffraction patterns similar to the diffraction patterns from decagonal quasicrystals were obtained from silicon specimens deposited onto mica substrates in the helium atmosphere [34] (it should be remembered that we considered here only the approximants of icosahedral quasicrystals). Despite the fact that one has to check whether this diffraction pattern is really formed due to a quasicrystal and not due to twins, we hope that this experiment would trigger new experimental studies of quasicrystals with tetrahedral coordination.

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